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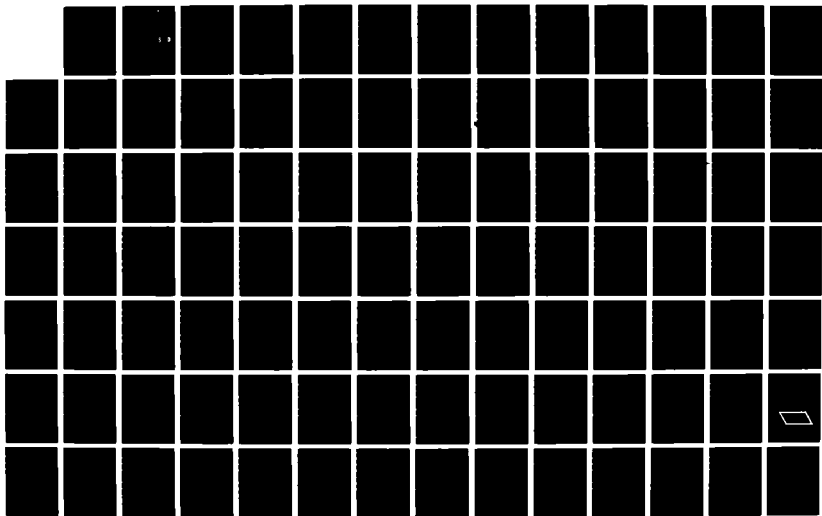
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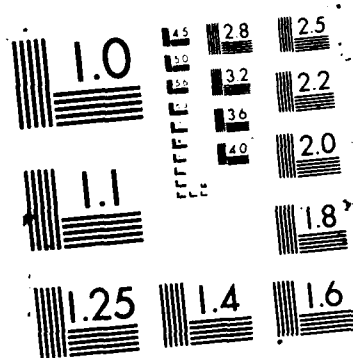
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The Pennsylvania State University

The Graduate School

Department of Meteorology

The Application of Vector Diffraction to the Scalar Anomalous  
Diffraction Approximation of van de Hulst

A Thesis in

Meteorology

by

Robert W. Mahood

Submitted in Partial Fulfillment  
of the Requirements  
for the Degree of

Master of Science

May 1987

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## ABSTRACT

The extinction, absorption, and differential scattering cross sections of particles are, in general, functions of the polarization state of the incident radiation; however, this dependency cannot be predicted by van de Hulst's anomalous diffraction approximation because it is a scalar theory. To overcome this deficiency, the Kirchhoff and Kirchhoff-Kottler vector diffraction formulations were used to modify anomalous diffraction in the hope that polarization effects could then be accounted for. Unfortunately, even with the modification, no polarization dependence was predicted for any of the cross sections. In actuality, the differential scattering cross section did show a second-order polarization dependence, but it was negligible within the limits of the approximation. In addition to the above work, a comprehensive, critical literature review of all previous uses of anomalous diffraction was conducted. In this review, the apparent differences between the Cross and Latimer (1970) and Stephens (1984) anomalous diffraction solutions for the extinction and absorption efficiencies of an infinite cylinder were reconciled.

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## INTRODUCTION

Exact solutions exist for determining the extinction and absorption of electromagnetic radiation by a few regular, homogeneous particles. Perhaps the best known of these are the Mie equations for spheres. While these solutions are valid regardless of the wavelength of the incident radiation, the particle's size, or its refractive index, they are frequently cumbersome; furthermore, we encounter few particles in nature which are regular and homogeneous. Consequently, we strive to find simpler limiting forms of these solutions. One limiting form which is useful for a wide range of particles of practical interest is the scalar anomalous diffraction approximation of van de Hulst (1957, Ch. 11). Although derived originally for spheres, it is readily applicable to many other shapes, and because of its simplicity, it can be applied to a system of particles without greatly complicating the resulting expressions.

Van de Hulst proposed the term "anomalous diffraction" to describe any theory based on the assumptions that (i) the particle is much larger than the wavelength of the incident light, and (ii) the complex relative refractive index of the particle is very nearly equal to one. The first assumption implies that we are in the geometric optics regime. The second assumption implies that rays are transmitted through a particle with little or no deviation and that essentially no energy is reflected.

In addition to the transmitted field, there is diffraction of the field by the particle according to Huygen's principle; this diffracted field can be adequately described in the Fraunhofer limit. It is the interference of the transmitted and diffracted radiation that is the foundation for the anomalous diffraction approach.

One question may quickly come to mind: How many particles of practical interest have relative refractive indices near one? The answer is "very few"; however, interestingly enough, the approximation provides the salient features of extinction for relative refractive indices as high as two. At visible wavelengths, the refractive indices of water droplets, ice crystals, and numerous biological particles lie between one and two; all of these particles are studied extensively. Consequently, I shall use the term light (by which I mean visible light) when referring to electromagnetic radiation unless otherwise specified. Although the theory is not restricted as such, I do this because visible light is the most commonly encountered form of radiation in studies utilizing anomalous diffraction techniques.

The purpose of this thesis is to first present a comprehensive, critical review of the literature on anomalous diffraction. Next, an attempt is made to extend the scalar approximation to include polarization effects. To do so, both the Kirchhoff and the Kirchhoff-Kottler vector formulations of Huygen's principle are used to modify the original relation. The new vector anomalous diffraction relation is then used to calculate the extinction efficiency and differential scattering cross section of a right circular cylinder to see if the method correctly predicts these functions' polarization dependence.

## Chapter 1

### REVIEW

#### 1.1 Overview

The anomalous diffraction approximation was first introduced by van de Hulst in his 1946 thesis; however, it did not come into widespread use until the publication of his now classic 1957 book. Being basically a combination of geometric optics and Fraunhofer diffraction, the approximation allows for the simple calculation of the extinction, absorption, and differential scattering cross sections for certain particles or groups of particles.

Van de Hulst coined the term "anomalous diffraction" to describe any theory based on the assumptions

$$x \gg 1 \quad (1)$$

and

$$|m-1| \ll 1 \quad (2)$$

where  $x = 2\pi a/\lambda$  is the size parameter,  $a$  is some characteristic dimension of the particle,  $\lambda$  is the wavelength in the medium, and  $m$  is the complex relative refractive index of the particle. The first assumption means that we are in the geometric optics regime; in other words, we can use ray tracing to represent light traversing the particle. The second assumption means that a ray is negligibly deviated as it crosses the particle's boundaries; in addition, because the Fresnel reflection coefficients vanish as  $m \rightarrow 1$ , little energy is reflected. Since  $m$  is complex, we can write it  $m = n - in'$ . The

assumption  $|m-1| \ll 1$  then means  $(n-1) \ll 1$  and  $n' \ll 1$ . Together, the assumptions imply that the scattered light will be confined to a narrow region about the forward (incident) direction.

It seems worthwhile here to make a point about the imaginary part of the relative refractive index. The assumption  $n' \ll 1$  will almost always be met by dielectrics at visible wavelengths ( $n' < 10^{-4}$  typically except in the region of an absorption band). However, a problem often arises with researchers' interpretations of  $n'$ . The value of  $n' = 6 \times 10^{-3}$  certainly meets the criterion  $n' \ll 1$ , yet many scientists will say that this value of  $n'$  implies weak absorption. A simple calculation will show that the absorption is far from weak.

For bulk matter, the Beer-Lambert Law says that the absorption of light is given by

$$I = I_0 \exp(-\alpha L) \quad (3)$$

where  $I$  is the irradiance (energy per unit area and time) at a distance  $L$  inside the medium,  $I_0$  is the incident irradiance, and  $\alpha$  is the absorption coefficient. The irradiance is also referred to as the intensity in some light scattering texts (Bohren and Huffman (1983) and van de Hulst (1957) for example). The absorption coefficient is related to  $n'$  by

$$\alpha = \frac{4\pi n'}{\lambda} \quad (4)$$

The inverse of  $\alpha$  gives an e-folding distance, i.e., the distance the light travels before being attenuated by  $e^{-1}$ . Stephens (1984) cites the

absorption implied by the value  $n' = 6 \times 10^{-3}$  as being weak. Substitution into (4) using red light ( $\lambda = 0.7 \mu\text{m}$ ) gives an e-folding distance of  $10 \mu\text{m}$ , thus  $1 \text{ mm}$  of this substance would decrease the incident radiation by a factor of  $e^{100}$ ! I doubt anyone would call this weakly absorbing. Consequently, I have several recommendations. First, I strongly suggest caution be exercised when using relative terms like weak or strong in reference to absorption; Stephens is far from being the only culprit. Second, I urge the use of physically real values of refractive indices. It may be simpler to conjure up some value that satisfies some desired specification, but it is much more enlightening if it corresponds to some real material. Lastly, it is necessary to explicitly state the wavelength when referring to absorption since the absorption coefficient depends explicitly on  $\lambda$  as well as  $n'$ . With the preceding points in mind, I will continue with the overview.

The anomalous diffraction approximation would probably be of only academic interest if it were not for the following fact: van de Hulst noticed that for spheres, the extinction efficiency's ( $Q_{\text{ext}}$ ) dependence on the parameter  $2x(m-1)$  was nearly identical to that of the exact theory even for  $n$  as high as two. The absolute value of  $Q_{\text{ext}}$  predicted by the approximation was somewhat different from that of the exact theory, however.

The approximation's greatest advantage is its simplicity; another is that  $Q_{\text{ext}}$  approaches its correct asymptotic value of two as  $x \rightarrow \infty$  for many particle shapes. Lastly, it is valid for a wide range of particle sizes; this fact makes it more appealing than the Rayleigh-Gans-Debye



(RGD) approximation which is based on the assumptions  $|m-1| \ll 1$  and  $2x|m-1| \ll 1$ . For spheres with real  $m$ , Moore et al. (1967) determined that the anomalous diffraction approximation was valid for  $x > 5$ ; however, for complex  $m$ , it proved valid even for  $x \approx 0.1$ .

The major disadvantage of anomalous diffraction is that it was developed from scalar postulates; therefore, polarization effects cannot be treated. Another disadvantage is that the magnitude of  $Q_{\text{ext}}$  predicted by the theory is smaller than that predicted by the exact theories as mentioned previously; however, Deirmendjian (1960) developed empirical corrections valid to within  $\pm 4\%$  for spheres. Lastly, the ripple structure given by the exact theories is not evident. This structure arises from such phenomena as surface waves and multipole resonances, so it is clear why the simple theory does not predict them. This drawback is not very significant for two reasons: first, for collections of particles, the ripple structure is smoothed out; second, for many applications, the ripple structure is simply a complicating nuisance.

In reference to the assumption  $x \gg 1$ , there is no apparent upper limit; in contrast, there must be some lower limit. Van de Hulst (1957) concluded using Huygen's principle that "... a pencil (of light) of width of the order  $p\lambda$  can lead on independent existence over a length  $p^2\lambda$ ." Bryant and Latimer (1969) interpreted van de Hulst's conclusion as follows: if a pencil of light is to traverse a thickness  $t$  of a particle, and if  $t = p^2\lambda$ , then the beam diameter must be at least  $p\lambda$ ; for a square area element  $\Delta A$  of edge length  $d$ , this gives  $d > (\lambda t)^{1/2}$  as the condition for applicability.

Van de Hulst (1957, Ch. 11) originally derived his theory for spheres. In the next section, I will derive the expressions for the extinction and absorption efficiencies and the differential scattering cross section of a homogeneous particle of arbitrary shape.

## 1.2 Application of Anomalous Diffraction to an Arbitrary Particle

Consider Figure 1 where the light is assumed to be incident from the  $-z$  direction. If  $t$  is the distance a ray travels through the particle, and if the surrounding medium is assumed to have  $m = 1$ , then the phase difference at  $P$  between a ray which traverses the particle and one which does not is

$$\Phi(\xi, \eta) = kt(\xi, \eta)(m-1) \quad (5)$$

where  $k = 2\pi/\lambda$  is the wave number, and  $\xi$  and  $\eta$  are rectangular coordinates in the plane  $V$ . If  $|m-1| \ll 1$ , the field is now known in all of the plane  $V$  which is near the particle. If the field is assumed to be unity outside of the geometric shadow region, then it is  $e^{-i\Phi}$  inside the shadow region. Thus, the field added to the original field is  $(e^{-i\Phi} - 1)$ .

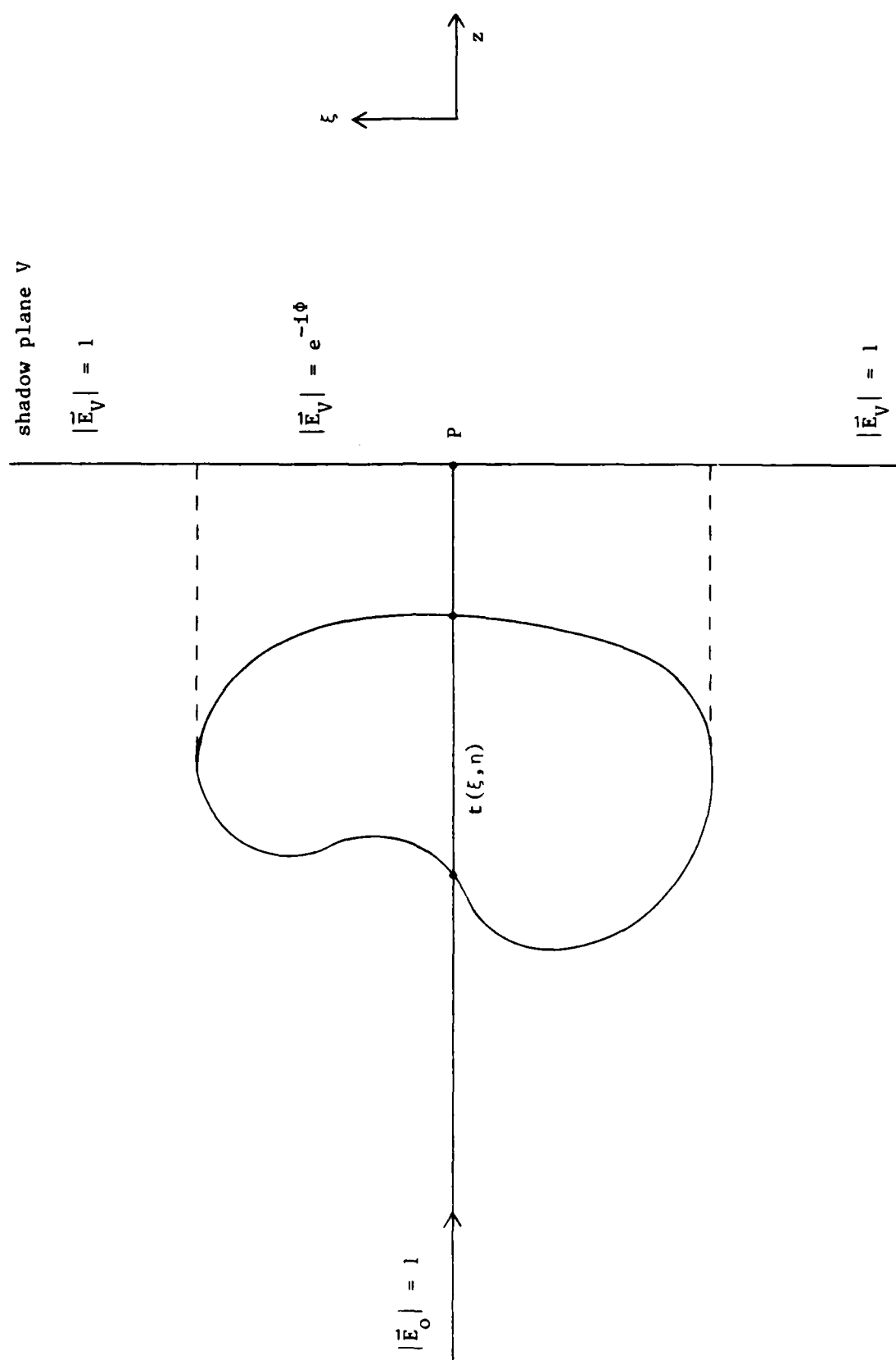
From the optical theorem, the extinction cross section is given by

$$C_{\text{ext}} = \frac{4\pi}{k^2} \text{Re}\{S(0)\} \quad (6)$$

where  $S(0)$  denotes the complex scattering amplitude in the forward direction, and  $\text{Re}$  means the real part. For an opaque body much larger than the wavelength, we find from Fraunhofer diffraction that

$$S(0) = \frac{k^2}{2\pi} G \quad (7)$$

Figure 1. The geometry to be considered when calculating the extinction and absorption efficiency of an arbitrary particle of refractive index  $|m-1| \ll 1$  embedded in a medium of real refractive index  $n = 1$ .



where  $G = \int_A d\xi d\eta$  is the area projected by the body onto a plane perpendicular to the incident direction. If we generalize (7) to include rays transmitted through the body, we get

$$S(0) = \frac{k^2}{2\pi} \int_G (1 - e^{-i\phi}) d\xi d\eta \quad (8)$$

The first term under the integral describes the diffracted field; the second term describes the transmitted field. The extinction then, is a maximum when the two fields interfere destructively. Substitution of (8) into (6) gives the extinction cross section.

The absorption cross section can also be calculated. If we recall that  $m = n - in'$ , the expression  $e^{-i\phi}$  contains a term  $e^{-ktn'}$  describing the amplitude decay. The intensity decay is just the square of this,  $e^{-2ktn'}$ ; therefore, the fraction of the incident intensity absorbed by the particle is  $(1 - e^{-2ktn'})$ . If we note that  $ktn' = \text{Re}\{i\phi\}$ , the absorption cross section can be written

$$C_{\text{abs}} = \int_G (1 - e^{-2\text{Re}\{i\phi\}}) d\xi d\eta \quad (9)$$

Next, we can calculate the extinction and absorption efficiencies; they are respectively

$$Q_{\text{ext}} = \frac{C_{\text{ext}}}{G} = \frac{2}{G} \text{Re}\left\{\int_G (1 - e^{-i\phi}) d\xi d\eta\right\} \quad (10)$$

and

$$Q_{\text{abs}} = \frac{C_{\text{abs}}}{G} = \frac{1}{G} \int_G (1 - e^{-2\text{Re}\{i\phi\}}) d\xi d\eta \quad (11)$$

Equations (10) and (11) are related to each other by

$$Q_{\text{ext}} = Q_{\text{abs}} + Q_{\text{sca}} \quad (12)$$

where  $Q_{\text{sca}}$  is the scattering efficiency; if  $m$  is real,  $Q_{\text{abs}} = 0$ , and thus  $Q_{\text{ext}} = Q_{\text{sca}}$ . If  $n' > 0$ , the asymptotic limit of  $Q_{\text{ext}}$  as  $x \rightarrow \infty$  is two. From (10), it is apparent that as  $Q_{\text{ext}} \rightarrow 2$ ,  $C_{\text{ext}} \rightarrow 2G$ ; in other words, an infinite, absorbing body removes twice as much energy from a beam as is geometrically incident on it. The two contributions of  $G$  to  $C_{\text{ext}}$  come one each from absorption and diffraction (scattering near the forward direction). For many shapes, such as spheres, cylinders, cubes, and discs, (10) and (11) can be solved analytically; for arbitrary particles, they must be numerically integrated.

Bryant and Latimer (1969) treated the arbitrary particle in a manner slightly different from that just outlined. In (5),  $\phi(\xi, n)$  may be a complicated function, especially for an irregularly shaped particle. Instead of the spatially varying  $\phi(\xi, n)$ , Bryant and Latimer suggested using an average phase shift defined by

$$\phi^* = kt_{\text{av}}(m-1) \quad (13)$$

where  $t_{\text{av}} = (\text{volume/projected area})$  is the average particle thickness. This approach provides a useful first guess as to how the particle will interact with the incident beam; however, a good deal of valuable information could be lost in such a crude averaging process. Also, the evaluation of  $t_{\text{av}}$  may be difficult since it will be a function of the particle's orientation in the beam. As a simple test, I compared the values of  $Q_{\text{ext}}$  obtained from both van de Hulst's and Bryant and

Latimer's methods for the case of a nonabsorbing sphere. Bryant and Latimer's method gave  $Q_{\text{ext}}$  values within about  $\pm 6-10\%$  of those obtained from van de Hulst's method. I suspect the disagreement may be stronger for a more complex particle. In light of the foregoing statements, I recommend  $\phi^*$  be used cautiously.

Once the extinction and absorption efficiencies of a single particle are known, attenuation by a collection of the particles can be calculated. We can use (3), but in order to distinguish between the single particle case and present case, I replace  $\alpha$  with  $\tau$  to get

$$I = I_0 \exp(-\tau L) \quad (14)$$

where  $L$  is now the distance into the (poly) dispersion. We can find  $\tau$  from

$$\tau = \int du \int d\gamma \int d\beta G(u, \gamma, \beta) Q_1(u, \gamma, \beta) n(u) g(\gamma) h(\beta) \quad (15)$$

where  $u$  is some parameter specifying particle size,  $\gamma$  and  $\beta$  are angles specifying particle orientation,  $n(u)$  is some size distribution function per unit volume, and  $g(\gamma)$  and  $h(\beta)$  are some angular distribution functions. If we let  $Q_1$  be  $Q_{\text{ext}}$ ,  $Q_{\text{abs}}$ , or  $Q_{\text{sca}}$ , then  $\tau$  becomes the extinction, absorption or scattering coefficient. Instead of the extinction coefficient, we may call  $\tau$  the turbidity. In the literature, I find that usually only one or two of the integrations in (15) are performed; for example, the integrations over all orientations may be evaluated for a system of randomly oriented particles of uniform size. Implicit in the use of (14) and (15) is the assumption that multiple scattering can be ignored. It is for a collection of particles that

anomalous diffraction is perhaps most useful; for regular particle shapes such as spheres and cylinders (15), does not become overly cumbersome to use. In fact, for some particle systems,  $\tau$  can be found analytically.

Van de Hulst (1957, p. 184) noted that the scattering amplitude function for small angles near the forward direction could be computed for spheres by adding a simple factor to  $S(0)$ . For an arbitrary particle which lacks the sphere's symmetry, a similar but slightly more complicated factor must be added.

Again, let the incident light be from the  $-z$  direction; also, let the origin lie somewhere within the particle. Furthermore, assume  $\xi$  and  $\eta$  are rectangular coordinates in the shadow plane and let the light be scattered at some arbitrary azimuthal angle  $\phi$  (measured from the  $+\xi$  axis) and some polar angle  $\theta$  (measured from the  $+z$  axis). We will require  $\theta$  to be small enough so that  $\sin \theta \approx \theta$ . Then, following van de Hulst's method for a sphere we find

$$S(\theta, \phi) = \frac{k^2}{4\pi} (1 + \cos \theta) \int_G (1 - e^{-i\phi}) e^{-ik\theta(\xi \cos \phi + \eta \sin \phi)} d\xi d\eta \quad (16)$$

for an arbitrary particle. The expression (16) agrees with that given by Meeten (1982b). Van de Hulst let the factor  $(1 + \cos \theta) = 2$  since  $\theta$  is small. Once  $S(\theta, \phi)$  is known, we can calculate the differential scattering cross section from

$$\frac{dC_{sca}}{d\Omega} = \frac{1}{k^2} |S(\theta, \phi)|^2 \quad (17)$$



where  $d\Omega$  is an element of solid angle. It is important to realize that  $dC_{\text{sca}}/d\Omega$  is not a derivative; rather it is written this way to remind us that it is the differential scattering cross section (Bohren and Huffman 1983, p. 72).

### 1.3 Literature Review

In the sections which follow, I will provide a comprehensive, critical review of all previous uses of anomalous diffraction. At the end of the chapter, I will provide reference tables listing  $Q_{\text{ext}}$  and  $Q_{\text{abs}}$ , when available, for each shape I have discussed. Several factors should be kept in mind while reading the literature review. First, the papers were reviewed on the basis of their use of anomalous diffraction; to consider all other factors would prove too lengthy for this thesis. Second, the notation given is that consistent with previous sections; in other words, I translated each author's notation into that of this thesis. Finally, the divisions I have created are not perfect; some papers may apply to several subsections. The categorization scheme I have chosen is the one which I considered to give the best mixture of fluidity and consistency.

#### 1.3.1 Spheres

The homogeneous sphere is the simplest particle shape to use in light scattering studies. It has no shape anisotropy; therefore, the extinction, absorption, and scattering efficiencies are polarization independent. I have found, probably because of its simplicity, that the sphere receives the most attention in the literature; this fact will become quite apparent if one notices that about 75% of this review is devoted to spheres.

### 1.3.1.1 Single Spheres

As mentioned earlier, van de Hulst first derived the anomalous diffraction approximation in his 1946 thesis, although he had not named it at that time. The approximation is often referred to by other names such as (i) the ray approximation, (ii) the van de Hulst approximation, and (iii) the soft particle approximation; the first and third could be confused with other approximations and should be avoided. The 1946 thesis is translated only fairly into English and is mostly of historical interest as the basis for van de Hulst's 1957 book. This 1957 text is a must for the newcomer to anomalous diffraction or light scattering in general. Included with van de Hulst's development of the approach for spheres (Ch. 11) are various limiting expressions for small and large phase shifts as well as expressions valid in the region of an absorption band. Table 1 gives van de Hulst's expressions for  $Q_{\text{ext}}$  and  $Q_{\text{abs}}$  for spheres and many other equivalent expressions.

Anomalous diffraction, as derived by van de Hulst (1957, Ch. 11), had its limitations. First, it underpredicted the magnitude of the exact value of  $Q_{\text{ext}}$ . Second, van de Hulst derived the theory only for spheres and normally incident, nonabsorbing cylinders. Third, effects of optical anisotropy were not considered; and lastly, polarization effects could not be predicted. In the remainder of this thesis, the attempts of various researchers to overcome these limitations are presented.

Many calculations have been performed comparing the exact values of  $Q_{\text{ext}}$  with the predictions of the anomalous diffraction approximation.

Penndorf (1956, 1959) made extensive calculations for real  $m$  and found van de Hulst's method useful for  $1 \leq n \leq 1.5$ . In 1956, Penndorf provided these simple correction factors for  $Q_{\text{ext}}^{\text{AD}}$ :

$$Q'_{\text{ext}} = \left[1 + \frac{n-1}{n} \frac{4.08}{\phi}\right] Q_{\text{ext}}^{\text{AD}} \quad 4.08 < \phi \quad (18)$$

$$Q'_{\text{ext}} = \left[1 + \frac{n-1}{n} \frac{\phi}{4.08}\right] Q_{\text{ext}}^{\text{AD}} \quad 5(n-1) < \phi < 4.08$$

Where  $Q'_{\text{ext}}$  is the corrected value, and  $Q_{\text{ext}}^{\text{AD}}$  is the value from anomalous diffraction. These corrections bring the results within 2% of exact values for  $1 \leq n \leq 1.5$ . A similar correction was offered by Klett (1984),

$$Q'_{\text{ext}} = \left[1.1 + \frac{(n - 1.2)}{3}\right] Q_{\text{ext}}^{\text{AD}} \quad (19)$$

with similar results for  $1 \leq n \leq 1.5$ . Deirmendjian (1960, 1969) extended Penndorf's corrections to include complex  $m$  for various ranges of  $\phi$ . His factors give  $Q'_{\text{ext}}$  within  $\pm 4\%$  of exact values. Deirmendjian (1960) also applied his correction factors to  $Q_{\text{abs}}^{\text{AD}}$ , but he did not specify the accuracy in this case; he did mention that the results may be up to 15% off in the region of an absorption band. In a continuance of his fine work, Deirmendjian et al. (1961) provided a minor section that graphically compared anomalous diffraction and Mie calculations of

$Q_{\text{ext}}$  for complex  $m$ . In his 1969 book (pp. 28-37), Deirmendjian expanded upon the results of the 1961 paper by including also a comparison of the values of  $Q'_{\text{ext}}$  obtained using his correction factors. Again, the comparison was for complex  $m$ , but unlike before, the results were presented in tabular form. Another paper in which a correction factor was offered for  $Q_{\text{ext}}^{\text{AD}}$  was that of Smart and Vand (1964); their complicated expression gives  $Q'_{\text{ext}}$  values within 2% of exact values for the range  $1 \leq n \leq 2.06$ . Smart and Vand's methods were difficult to follow. For example, they introduced the transmission coefficient at normal incidence into van de Hulst's expression for  $Q_{\text{ext}}^{\text{AD}}$ , although they did not identify it as such. Their logic for adding the factor was vague; in fact, I would think the factor should be added twice if at all: once to include rays entering the sphere and once to include rays exiting it. Regardless, Smart and Vand used their correction to isolate the ripple structure associated with the exact theory by taking  $|Q_{\text{ext}}| - |Q'_{\text{ext}}|$ . This application, at least, was a novel use for anomalous diffraction. Kerker (1969) gave a fine review of anomalous diffraction for spheres (pp. 104-127), cylinders (pp. 291-293), cubes (p. 127), and spherical polydispersions (pp. 454-457). He provided both Deirmendjian's (p. 126) and Smart and Vand's (pp. 113-114) correction factors; however, he failed to identify a variable in his section on Smart and Vand. In Kerker's equation 4.2.12,  $Q_{\text{sca}}(1)$  is simply  $Q_{\text{ext}}^{\text{AD}}$  for  $n' = 0$ . Also note that the third term in Kerker's equation 4.2.27 is missing a factor of  $\rho^{-1}$ ; this equation gives  $Q_{\text{ext}}^{\text{AD}}$  for absorbing spheres (see Table 1). If we continue the review of those papers comparing anomalous diffraction predictions with those of Mie theory,

we find a nice, concise paper by Moore et al. (1968). They provided excellent graphs of  $Q_{\text{ext}}^{\text{AD}}/Q_{\text{ext}}^{\text{Mie}}$  versus  $x$  and  $Q_{\text{abs}}^{\text{AD}}/Q_{\text{abs}}^{\text{Mie}}$  versus  $x$ . A similar treatment was performed using the RGD approximation. From their comparisons, Moore et al. determined that for  $n' = 0$ , anomalous diffraction was valid for  $x > 5$ ; however, for  $n' \neq 0$ , it remained valid even for  $x \approx 0.1$ . Also in 1968, Farone and Robinson, in an often-cited paper, mapped the regions of the  $m$ - $x$  domain in which anomalous diffraction was within 15, 50, and 100% of exact Mie results. They considered the ranges  $1 \leq x \leq 20$  and  $1.1 \leq n \leq 2.5$ ; furthermore, they included small angle light scattering as well as  $Q_{\text{ext}}$ . Although the paper has valuable information, its terminology is poor, and the nominal assumptions listed for the anomalous diffraction approximation are incorrect. Farone and Robinson gave  $|m-1| \ll 1$  and  $x|m-1| \ll 1$  as the assumptions required for van de Hulst's method; these are actually the assumptions of the RGD approximation. In addition to this mistake, they made statements such as "Rayleigh-Gans scattering occurs when . . . ;" Rayleigh-Gans is a theory which predicts light scattering, not a form of light scattering. I believe great difficulties may arise when we fail to separate reality from descriptions of it. The last comparison paper for spheres is that of Debi and Sharma (1979). Not only did they compare anomalous diffraction to the Mie theory, they compared it to the RGD and Eikonal approximations as well. I find this paper very useful if one wishes to find the best approximation for a given situation. Debi and Sharma considered only real  $m$  with  $1.05 \leq n \leq 1.30$  and  $0.2 \leq x \leq 25$ . Of four  $m$ - $x$  domains they identified, anomalous diffraction was the best approximation in two:  $x > 1, \phi > 4$  and  $0.4 < x < 1.2, \phi < 1$ .

The Eikonal approximation was strongly promoted by Debi and Sharma. It applies to the same  $m$ - $x$  domain as anomalous diffraction, and in fact, is in all ways identical to anomalous diffraction except for the phase shift. In the Eikonal approximation, the phase shift is given by

$$\phi_E = \frac{1}{2} (m+1) \phi_{AD} \quad (20)$$

where the subscripts refer to the Eikonal and anomalous diffraction approximations, respectively. Since  $|m-1| \ll 1$  is assumed, the Eikonal approximation is nearly equal to the anomalous diffraction approximation; moreover, they become identical as  $m \rightarrow 1$  for real  $m$ . Van de Hulst's approximation is more heavily used by, and more familiar to those who study light scattering, so I see no real reason or advantage in considering the Eikonal approximation. I hope Debi and Sharma perform a similar study for complex  $m$  in the future as the results may be interesting.

In contrast to the comparison papers, several researchers were content to use van de Hulst's sphere approximation to gain insight into more difficult scattering problems. In an excellent, short letter, Latimer and Bryant (1965) eliminated any possible ambiguity in the notation van de Hulst used in his original derivation; subsequently, they developed expressions for the phase shifts in absorption bands of the Lorentzian or Gaussian type. These phase shifts could then be used in anomalous diffraction expressions. Plass (1966) went on to systematically explore the dependence of  $Q_{ext}^{AD}$  and  $Q_{abs}^{AD}$  on  $m$  by varying  $n$  and  $n'$  incrementally. Assuming the exact values of  $Q_{ext}$  and  $Q_{abs}$

have the same functional dependence, Plass made some interesting observations. Plass, however, is another person who may have misinterpreted the meaning of  $n'$ ; for example, he called  $n' = 0.01$  small absorption. For visible light, this value of  $n'$  implies enormous absorption. Next, in a fine 1969 paper, Bryant and Latimer illustrated numerical integration techniques for determining  $Q_{\text{ext}}$  in which a sphere was modeled as a collection of concentric cylinders. Each cylinder's scattering was described in terms of anomalous diffraction. This method can readily be applied to a coated sphere over which  $m$  does not vary too greatly. In a more complex departure from van de Hulst's simple expressions, Meeten (1982b) generalized anomalous diffraction to describe small angle light scattering by anisotropic spheres. His results might be of great value as he gave the scattering matrix in terms of the particle's Jones matrix; the components of the scattering matrix are each derived from an anomalous diffraction approach. Thus, polarization effects can be considered for an anisotropic sphere. Meeten's approach leaves me with some doubts. Meeten made two important assumptions, one completely intuitive, that while logical, have no physical basis. I believe some of his results could be realized by other means; consequently, this paper warrants further study. Finally, a recent paper by Klose (1986) appeared to have important results. From a completely different approach, without the use of the forward scattering amplitude, Klose derived expressions for  $Q_{\text{ext}}$  identical with those of anomalous diffraction for a sphere, cylinder, and spheroid. Furthermore, Klose reported a polarization dependent extinction efficiency for the spheroid, something not appearing in the anomalous

diffraction results. However, I could not understand why no polarization dependence was found for the cylinder; after all, a highly prolate spheroid is often used to represent a cylinder. Thus, I wrote to Klose about this apparent conflict. Upon checking, Klose found an error in his equation 2.20 for the spheroid; upon correction, the polarization effects no longer appeared for the spheroid. Although expected, this result is unfortunate. Klose assured me that he would publish an errata soon. Klose's paper is difficult to follow, but the fact that he duplicated van de Hulst's results in a completely independent manner is interesting. Since Klose's method is far more complicated than that of van de Hulst, I do not foresee it having any great practical value.

#### 1.3.1.2 Monodispersions

Although few papers addressed spherical monodispersions and their associated features, not surprisingly, all of the ones I found were concerned with colloidal suspensions. Champion et al. (1978) derived the refractive index increment  $dn/dc_2$ , where  $c_2$  is the concentration of the dispersed phase, for dilute dispersions using the Rayleigh, RGD, and anomalous diffraction approaches. In addition to spheres, they also considered discs which prompts me to state the following opinion: Champion et al. called "Mie scattering" that for particles of the order  $x = 1$ ; however, since Mie developed his relations for spheres, I believe the term "Mie" should only be used in reference to spheres. Also, as I mentioned in my review of Farone and Robinson (1968), I dislike terms such as "Mie scattering" and "Rayleigh-Gans scattering" because neither is a form of scattering. I realize phrases like this are common in the



literature, but I think my point is valid. I will not address this issue again. To continue, Champion et al. found that the refractive index increment, unlike  $Q_{\text{ext}}^{\text{AD}}$ , could be extrapolated correctly from the anomalous diffraction size region to the Rayleigh region. The Rayleigh approximation is valid for particles with  $x \ll 1$  and  $|mx| \ll 1$ . In a continuance of their work, Champion et al. (1978b) discussed the refraction of light by a dilute suspension of spheres, they used the exact Mie theory as well as the Rayleigh, RGD, and anomalous diffraction approximations. Next, Champion et al. (1979b) compared refraction and extinction (by which they meant  $Q_{\text{ext}}$ ) to find the similarities and differences. For the comparison, they defined a term  $P_{\text{ref}}$ , the refraction efficiency in analogy to  $Q_{\text{ext}}$ ; I found  $P_{\text{ref}}$  a more difficult concept to understand physically. Nevertheless, the paper was simple with potentially important results. Champion et al. found that a refractometric method would be better for sizing larger particles than a turbidimetric method. In all cases I have encountered, turbidimetric methods were used as the sizing technique. Therefore, the Champion et al. conclusions merit further study.

Meeten (1980a, 1980b) performed a simple, yet clever generalization of anomalous diffraction to enable the calculation of the linear birefringence and linear dichroism of a dispersion of colloidal particles. In Meeten (1980a), the generalization could apply to any anisotropic particles as long as all of their optic axes were aligned, but alignment of the optic axes is an unrealistic requirement. Meeten (1980b) overcame this restriction by allowing for arbitrarily oriented, anisotropic spheres. Meeten's (1980a) simple approach is worth

repeating here. Suppose a particle has mutually orthogonal optic axes  $a$ ,  $b$ , and  $c$  with refractive indices  $m_a$ ,  $m_b$ , and  $m_c = m_b$ , respectively. Meeten assumed that upon transmission, the phase lag of light polarized parallel to the  $a$  or  $b$  axes could be described by

$$\phi_e = ktm_1 (\mu_a - 1) \quad (21)$$

or

$$\phi_o = ktm_1 (\mu_b - 1) \quad (22)$$

respectively, where  $\phi_e$  is the phase lag of the extraordinary ray,  $m_1$  is the refractive index of the continuous phase,  $\mu_a = m_a/m_1$ ,  $\phi_o$  is the phase lag of the ordinary ray, and  $\mu_b = m_b/m_1$ . Meeten then separately applied (21) and (22) to (8) to give  $S(0)_e$  and  $S(0)_o$ . Meeten's results confirmed the empirical Zocher's rule which states that linear dichroism is a maximum when linear birefringence is a minimum. Although clever, these results lack experimental verification. Meeten (1982a) pointed out the following error in Meeten (1980b): in equations (5) and (30), the right-hand side must be divided by  $4\pi\epsilon_0$  where  $\epsilon_0$  is the permittivity of free space.

Latimer and Wamble (1982) found another good use for anomalous diffraction. They wanted to qualitatively model the observed modifications in scattered light fluxes due to the aggregation of colloidal particles. The aggregates are complex in shape, yet some shape information is lost through the randomness of their orientations. Anomalous diffraction, with its attention to gross particle parameters, seemed a useful tool for the study; it was unnecessary to complicate things with exact theories since no exact theory wholly applied.

Latimer and Wamble chose the coated sphere as a model for the aggregation. The refractive index and volume of the coat matched those of the colloidal particles in the aggregation; the refractive index and volume of the core matched those of the interparticle spaces in the aggregation. The paper is good overall with two exceptions: first, the section on information theory consists of mostly "hand-waving" arguments and second, the scales of Figures 9 and 10 are different thus giving the appearance of better quantitative agreement between experiment and theory than might actually exist.

#### 1.3.1.3 Polydispersions

Polydispersions are the rule rather than the exception in naturally occurring collections of particles. The variables of interest when considering polydispersions are  $\tau$ , the turbidity, and  $\bar{Q}_{\text{ext}}$ , the extinction efficiency of the polydispersion. This latter quantity is simply  $\tau$  divided by the total geometric cross section per unit volume,  $\bar{G}$ . For spheres,  $\bar{G}$  is given as

$$\bar{G} = \int_0^{\infty} \pi a^2 n(a) da \quad (23)$$

where  $a$  is a sphere's radius. By replacing the exact values of  $Q_{\text{ext}}$  and/or  $n(a)$  in (15) and (23) with analytic functions, we can hope to analytically integrate or at least simplify the expressions for  $\tau$  and  $\bar{Q}_{\text{ext}}$ . While these analytic expressions may be less realistic physically, they can allow us to find the characteristic dependencies of  $\tau$  and  $\bar{Q}_{\text{ext}}$  on particle size or refractive index for example. In this section, the analytic expressions used to replace the exact value of

$Q_{\text{ext}}$  in (15) are those for spheres with real or complex  $m$  derived from the anomalous diffraction approach (see Table 1).

Van de Hulst (1957, p. 194) illustrated the calculation of  $\bar{Q}_{\text{ext}}$  for three simple, yet unrealistic size distributions. A more physically acceptable approach was undertaken by Zuev et al. (1965). They calculated  $\bar{Q}_{\text{ext}}$  using Deirmendjian's corrected value of  $Q_{\text{ext}}^{\text{AD}}$  as the kernel in the turbidity relation. For a size range  $2 \leq a \leq 10 \mu\text{m}$  and with  $0.5 \leq \lambda \leq 14 \mu\text{m}$ , Zuev et al. tested their calculations by collecting experimental data from an artificial fog with a  $\gamma$  size distribution. The graphs depicting the experimental versus theoretical values of  $\bar{Q}_{\text{ext}}$  were almost impossible to decipher; however, upon close examination, the values are seen to be in reasonable agreement.

Deirmendjian (1959, 1960) calculated the turbidity at the surface due to water droplets in the atmosphere using several haze and cloud models. In the first study, Deirmendjian (1959) ignored absorption by considering only  $0.8 \leq \lambda \leq 2.25 \mu\text{m}$  where water shows few strong absorption bands. In the follow-up study, Deirmendjian (1960) was forced to consider absorption since he was interested in the region  $2.25 \leq \lambda \leq 14 \mu\text{m}$ . Water shows several strong absorption bands in this wavelength range. Although in the first paper Deirmendjian used exact Mie values, in the subsequent one he used his corrected values of  $Q_{\text{ext}}^{\text{AD}}$  in the turbidity relation. Since  $m$  is strongly wavelength dependent in this part of the spectrum,  $Q'_{\text{ext}}$  was calculated at many individual wavelengths. For a further analysis of the extinction by spherical polydispersions, I recommend Deirmendjian (1969). In a similar study, Hilbig (1965/66) calculated the turbidity of a Maxwell-distributed

collection of nonabsorbing spheres using  $Q_{\text{ext}}^{\text{AD}}$  as the kernel of the turbidity relation. Since Hilbig's paper was unavailable in English, I have provided only the information from his abstract. Next, Casperson (1977), in an outstanding paper, developed relatively simple analytic expressions for  $\tau$  using  $Q_{\text{ext}}^{\text{AD}}$  with real or complex  $m$  in (15). The size distribution was modeled as being either logarithmic or power-law-exponential. These size distributions are frequently used to model clouds, rain, and atmospheric aerosols. Casperson was all-encompassing in his analysis and quite realistic about his results. He made the following valuable point which should be considered by all who perform turbidity calculations using anomalous diffraction:  $Q_{\text{ext}}$  is small for small  $x$  (i.e.,  $x < 1$ ) when  $|m-1| \ll 1$ , so the extinction will be dominated by the larger particles; consequently, the fact that anomalous diffraction is poor for  $x < 1$  will be of little importance.

Lastly, Yamamoto and Tanaka (1969), Box and McKellar (1978a) and Fymat and Mease (1978) all found anomalous diffraction to be an excellent tool for gaining insight into the inverse problem of light scattering. I will elaborate on the inversion problem in another section (1.3.1.5). Basically, in inversion problems, we use measured values of  $\tau(\lambda)$  and invert the turbidity relation to find parameters of the particle system like the size distribution or refractive index. For their inversions, all three groups used exact Mie theory to calculate  $Q_{\text{ext}}$  in (15). However, each group replaced  $Q_{\text{ext}}$  with  $Q_{\text{ext}}^{\text{AD}}$  to study the direct problem. By studying the direct problem, insight may be gained into the potential pitfalls of the inverse problem. First, Yamamoto and Tanaka (1969) were concerned with the size distribution of atmospheric

aerosols. They ignored absorption by citing a study in which the refractive index of the aerosols was given as  $m = 1.5 - 0.01i$  or  $m = 1.5 - 0.1i$ ; they declared that  $n'$  decreased for a moistened aerosol. For the region  $0.35 \leq \lambda \leq 2.27 \mu\text{m}$  which they considered, even if  $n'$  of a moistened aerosol decreased by a factor of 10 (especially if  $n' = 0.1$ ), I do not think that ignoring absorption was wise here. Regardless, Yamamoto and Tanaka used  $Q_{\text{ext}}^{\text{AD}}$  in the turbidity relation as a check of the dependence of  $\tau$  on  $n$ . In this way, they could estimate the error incurred if their assumed value of  $n = 1.5$  was incorrect. Next, Box and McKellar (1978a), armed with a knowledge of the column-integrated turbidity's dependence on refractive index, were well prepared to attain their goal: the determination of atmospheric aerosol columnar loading from measurements of  $\tau(\lambda)$ . Please note that their  $n(a)$  is the size distribution per unit column area unlike mine which is per unit volume; consequently, their  $\tau$  is dimensionless. Likewise, Fymat and Mease (1978), armed with a knowledge of the turbidity's dependence on refractive index, were better prepared to attain their goal: the retrieval of the complex refractive index of atmospheric aerosols using narrowband spectral transmission ratios. In closing this section, I must make two comments on Fymat and Mease's paper. First, their graphs of  $Q_{\text{ext}}^{\text{AD}}$  versus  $a$  were confusing because their choice of ordinate and abscissa was the opposite of that normally encountered. Second, for a portion of their study, Fymat and Mease considered  $n' \geq 0.1$  which may be in violation of the anomalous diffraction assumption requiring  $n' \ll 1$ ; the approximation is poor for  $n' \geq 0.1$  and should not be accepted as an accurate approximation to Mie theory in these cases.

#### 1.3.1.4 Biological particles

In the past 25 years, biologists have become more aware of the value of light scattering as a nondestructive tool for acquiring information on cell cultures. I am devoting a special section to the treatment of biological cells because they present a unique problem. Since a cell is a highly intricate, heterogeneous system, we cannot hope to exactly predict how a given cell will scatter light; in fact, because of the complexity, one might think it impossible to predict the scattering at all. Yet, as we will see in the forthcoming discussion, fairly accurate light scattering predictions can be made. The success of these predictions can be attributed to the loss of light scattering detail inherent in a randomly oriented dispersion of cells. As a reminder, all researchers in this section have modeled their cells as being spherical. The light scattering predictions are derived from the Mie theory, the RGD approximation, and most importantly to this thesis, the anomalous diffraction approximation.

My recommended starting point for those interested in light scattering techniques for cells is Latimer (1982). In this excellent paper, he provided a review of the uses, potential uses, and limitations of light scattering theory for deriving information from cell samples. He discussed the Mie theory, the RGD approximation, and the anomalous diffraction approximation and noted that most cells are of such a size and composition, that in studies using visible light, the latter two approximations usually apply. Latimer pointed out that the overall cell is usually in the large particle domain with an inner structure in the small particle domain; consequently, extinction and small angle light

scattering should be used to investigate the gross cell structure while large angle light scattering should be used to investigate the microstructure of the interior.

The first paper to appear on this section's subject was that of Latimer and Rabinowitch (1959). They used van de Hulst's (1957, p. 191) anomalous diffraction expressions for extinction in the region of an absorption band to predict the experimentally observed enhanced scattering on the long wavelength side of an absorption band. The particle of interest was Chlorella, and the absorption was due to chlorophyll pigment. The pigment was modeled as being uniformly distributed throughout the cell. Although a simple approach, the observed characteristics of the scattering were predicted. In a follow-up study, Charney and Brackett (1961) tried an empirical correction to  $\phi$  in van de Hulst's (1957, p. 175) expression for  $Q_{\text{ext}}^{\text{AD}}$  for spheres. Their modified  $\phi$  had two terms: the first was proportional to the refractive index of the cell relative to the surrounding medium; the second was proportional to this same refractive index adjusted by the strongly wavelength dependent pigment refraction. Charney and Brackett were well aware of the high degree of approximation inherent in their approach, yet they achieved excellent agreement between their theoretical predictions and experimental observations of the light scattering by Chlorella.

Since absorbers (pigments) are often only a small portion of a cell, and because of the large intracellular distances, some light passes through a dispersion virtually undamped. This effect causes distortions in the measurements of absorption spectra when some



conventional spectrophotometers are used. Latimer and Eubanks (1962) termed this effect the "sieve" effect and sought a correction for it. Their correction was based on a minor modification of van de Hulst's (1957, p. 181) expression for  $Q_{abs}^{AD}$ . Latimer (1967) further refined the method. Like Charney and Brackett (1961), even with the many approximations they used, Latimer and Eubanks obtained absorption spectra for red blood cells and chloroplasts in good agreement with previously published spectra.

Latimer et al. (1968) made a theoretical investigation of how conformational changes in a cell's structure affects light scattering. They made two basic assumptions. In the first, the cell was assumed to take up or extrude water with no change in dry weight; in the second, the cell's interior was assumed to behave like an ideal solution. For an ideal solution, the refractive index is modeled as being inversely proportional to the system's volume so that we can write the phase lag of transmitted light in the shadow plane as

$$\phi = kt (m_o - 1) V_o / V \quad (24)$$

where  $m_o$  and  $V_o$  are the initial values of refractive index and volume, respectively. By substituting this  $\phi$  into the expression for  $Q_{ext}^{AD}$ , the effect of volume changes becomes fairly simple to understand physically. Within the limits of the approximation, shrinkage decreases the cell's projected area and thus decreases extinction; on the other hand, shrinkage increases the effective refractive index and thus increases extinction. Since the two effects compete, it is not obvious beforehand

whether a given change will increase or decrease extinction; it will depend on the cell's original size, refractive index, and the wavelength of the incident beam. Once the nature of the problem was known, more precise calculations were performed. Bryant et al. (1969b) experimentally confirmed the predictions of Latimer et al. (1968) using exact Mie calculations for the theoretical work. Comparison was also made to the predictions of anomalous diffraction and the RGD approximation. Only anomalous diffraction was in qualitative agreement with both the Mie theory predictions and experimental observations.

Bryant et al. (1969a) measured  $C_{\text{ext}}$  of E. Coli cells, yeast cells, and spinach chloroplasts. These measured values of  $C_{\text{ext}}$  were compared with calculated  $C_{\text{ext}}^{\text{AD}}$  values. The particle parameters such as size, shape, and refractive index were obtained experimentally and used in the theoretical calculations. Initially, all cells were modeled as spheres; subsequently, calculations were made in which the yeast cells and spinach chloroplasts were modeled as spheroids and in which the E. Coli cells were modeled as infinite cylinders. For both the spheroid and cylinder cases, the theoretical predictions were in better agreement with experimental observations than those of the sphere cases. For spheroids of axial ratio close to one, the effect of asphericity was found to be almost negligible. In contrast to the excellent predictions of the models of E. Coli and yeast cells, an artificially low value of  $m$  had to be used for the spinach chloroplast to get good agreement between theory and observation; no reason was offered. Bryant et al. contained a lengthy, albeit poor dissertation on the physical principles underlying the anomalous diffraction approximation. For example, they

used phrases like "light bounces" and "light bends"; I think these metaphors are suitable only in elementary texts. Latimer (1983) resolved an apparent conflict between the results of the previous work, Bryant et al. (1969a), and those of Bussey (1974). Contrary to Bryant et al., Bussey found decreased transmission through a collection of yeast cells upon shrinkage. Bussey's theoretical work was based on an expression derived from anomalous diffraction in the limit of small phase shifts; however, his cells were too large for this relation to apply. Also, the parameter Bussey needed to measure could not be obtained correctly with the photocell he used. Fortunately for Bussey, his two errors compensated each other; as a result, his theoretical and experimental transmission values were incorrectly in good agreement.

Morris and Jennings (1977) used anomalous diffraction to obtain closed-form, analytic expressions for small angle light scattering by coated spheres. The success of their method was dependent on the sphere being either very thickly or very thinly coated. Morris and Jennings noted that many cells could be modeled by a thinly coated sphere. Their paper was well done and concise; only their research on previous uses of anomalous diffraction was lacking. Morris and Jennings claimed little use had been made of van de Hulst's approximation, a fact easily disputed by the length of this literature review.

Morel and Bricaud (1981) used a theoretical approach to reinvestigate the problem of absorption in a discrete medium and the applicability of the Beer-Lambert Law in such cases. They showed that the concept of specific absorption, the absorption per unit absorber concentration, had to be modified for a discrete medium. Morel and

Bricaud were concerned with algal cells; they modeled them as homogeneous spheres and applied van de Hulst's (1957, p. 181) expression for  $Q_{abs}^{AD}$  to them. Although they used anomalous diffraction, they did so with virtually no discussion of its basic precepts. When using an approximation, all of the premises should be stated so that the reader is aware of the applicability of any resulting theory. The choice of anomalous diffraction was wise here as the whole study was very approximate. Why bother making exact scattering calculations for a first guess theory? Morel and Bricaud found three basic regimes. For small and large phase shifts, the specific absorption was nearly constant, so the Beer-Lambert Law was valid. Between these regions, the specific absorption was variable, so the Beer-Lambert Law did not strictly apply. Morel et al. (1983) continued to make good use of anomalous diffraction, although I had to check Morel and Bricaud (1981) to even know they were using it. Bricaud et al. measured absorption and scattering coefficients of four oceanic phytoplanktons and transformed the coefficients into specific coefficients and optical efficiencies. A knowledge of  $Q_{abs}$  for phytoplanktons is valuable for determining photosynthetic yields. For a theoretical investigation, they assumed the phytoplankton to be homogeneous spheres, then anomalous diffraction was used to calculate  $\bar{Q}_{sca}$  and  $\bar{Q}_{abs}$ , the scattering and absorption efficiencies of the entire systems, for various size distributions and refractive indices. The graphs of these results are superb. As a final comment, the notation used in the paper was that proposed by the International Association for Physical Sciences of the Ocean (IAPSO); I find this notation terrible. In my opinion, attempts to impose

standardized notations, while laudable, are usually failures, and the readability of papers and texts suffers as a result. Another paper following the IAPSO guidelines, and the last of this section, is that of Bricaud and Morel (1986). Like their previous work, they used anomalous diffraction with little explanation of the underlying assumptions or accuracy of the approximation. Again, phytoplankton were modeled as homogeneous spheres. As inputs to their anomalous diffraction-based calculations of  $\bar{Q}_{sca}$  and  $\bar{Q}_{abs}$ , they used the experimentally determined size distribution, measured absorption spectra, and an adjustable real refractive index  $n$  of the form  $n = 1 + \epsilon$  where  $\epsilon$  is some small number. Even though Bricaud and Morel admitted that their whole approach was just a first approximation, the agreement between theoretical predictions and experimental observations was fair; the graphs depicting this comparison were small, crowded, and hard to read, however.

#### 1.3.1.5 Inversion techniques

All of the sections thus far have dealt with the direct problem of light scattering; in this section, we turn our attention to the "harder" indirect problem. Bohren and Huffman (1983, p. 10) provided the following useful analogy: the direct problem is like trying to predict what a known dragon's tracks look like; the indirect problem is like trying to predict what an unknown dragon looks like from an inspection of its tracks.

##### 1.3.1.5.1 Monodispersions

For a monodisperse system of spheres the turbidity relation reduces to

$$\tau = \pi a^2 N Q_{ext} \quad (25)$$

where  $N$  is the number of particles per unit volume. By experimentally measuring  $\tau$  and  $N$ , and by substituting  $Q_{\text{ext}}^{\text{AD}}$  for the exact value, it becomes relatively straightforward to invert (25) to get the sphere radius,  $a$ , or refractive index,  $m$ , if either is known beforehand. Please note that absorption is neglected in each of the papers of this section.

Shchegolev and Klenin (1970) developed a system of equations, one derived from (25), that allowed for the simultaneous determination of both  $a$  and  $m$ . The inputs to the system of equations were  $\tau(\lambda)$  measured over a narrow wavelength spectrum and  $(\tau/N)_0$ , the specific turbidity extrapolated to infinite dilution. The use of anomalous diffraction was well hidden in this paper, although I do not know why since the theoretical predictions matched the experimental observations fairly well. Next, Shchegolev and Klenin (1971) found that the relation for the wave exponent,  $w$ , given by

$$w = \frac{\partial \ln \tau}{\partial \ln \lambda} = \frac{\phi}{Q_{\text{ext}}} \frac{\partial Q_{\text{ext}}}{\partial \phi} \quad (26)$$

could be expressed analytically if  $Q_{\text{ext}}^{\text{AD}}$  was substituted for the exact value. The resulting predictions of  $w$  agreed well with previously published literature values. Shchegolev and Klenin illustrated the usefulness of anomalous diffraction rather nicely here. Finally, Klenin and Shchegolev (1971) put the theory of their previous two papers to work in the area of polymer science. They found, within certain restrictions, that the mass of polymer precipitated during turbidimetric

titrations could be calculated from a knowledge of the turbidity variation which occurred.

The last paper of this section is that of Sharma and Debi (1980). In this difficult to follow paper, the effects of using anomalous diffraction, the RGD approximation, or the Eikonal approximation were compared for the determination of sphere size and weight by inversion methods. Sharma and Debi investigated the ranges  $1 \leq x \leq 25$  and  $1.05 \leq n \leq 1.30$ . For spheres of  $x \geq 1$  and  $m \leq 1.10$ , anomalous diffraction was the most useful approximation.

#### 1.3.1.5.2 Polydispersions

The fundamental task of this section is to invert the turbidity relation for spheres,

$$\tau = \int_0^{\infty} \pi a^2 Q_{\text{ext}}(\lambda, m) n(a) da \quad (27)$$

so that  $n(a)$ , the size distribution function, can be found. The accurate, remote, and nondestructive determination of  $n(a)$  is of great interest to scientists studying atmospheric aerosols, colloidal suspensions, and cell cultures to name just a few. The method of this section is to first replace the exact kernel,  $Q_{\text{ext}}$ , with the approximate  $Q_{\text{ext}}^{\text{AD}}$ . Except where otherwise noted, the kernel  $Q_{\text{ext}}^{\text{AD}}$  applies only to nonabsorbing spheres. I attribute the minor attention given to absorbing spheres to the fact that the inversion of (27) is quite complicated even when ignoring absorption. The next step of the method is to measure the data function,  $\tau$ , over a wide wavelength spectrum. The collective data set,  $\tau(\lambda)$ , is then usually referred to as the multi-spectral extinction.

Equation (27) is a Fredholm integral equation of the first kind; the inversion of such relations is an example of an ill-posed problem.

I quote the excellent introduction of Viera and Box (1985):

Such [ill-posed] problems fail to fulfill one (and often all three) of the following conditions: (i) existence of a solution (ii) uniqueness of a solution, and (iii) continuity of the solution on the data function. Ill-posedness leads to a loss of information and to highly unstable solutions: that is, small changes in the data function (such as will always arise from experimental error) can produce very large changes in the solution. (p. 4525)

With few exceptions, the papers of this section can be attributed to three groups of researchers: (i) Shifrin and/or Perelman and their associates, (ii) Box and McKellar and their associates, and (iii) Fymat and his associates. Each of these groups attempted, with varying degrees of success, to overcome the difficulties outlined in the previous paragraph. I will present each group's work in the order listed above, which is in order of increasing simplicity of method, and follow these with the remaining works.

The material available from the Shifrin-Perelman group all originated in the Soviet Union between the years 1961 and 1980. I found that the often poor quality of the Russian-to-English translations hampered my ability to glean information from the articles; however, translations aside, I also noted that the papers were presented in a most unsatisfactory manner. First, many papers were written where a few would have sufficed; the change from paper to paper was frequently minor. Additionally, most of the papers extensively and necessarily cross-referenced previous ones in the series. The necessity of the cross-referencing arose from the fact that each paper was much too far



from being self-contained; especially for the early papers, it was virtually impossible to follow a given paper without all previous ones at hand. Fortunately, the cross-references gave the exact location of an item; however, many bibliographies in the series lacked page numbers in their citations thus making it more difficult to locate a given reference. Another major problem with the group's work was that they rarely discussed the implications associated with replacing  $Q_{\text{ext}}$  by  $Q_{\text{ext}}^{\text{AD}}$ . Also along this line, it was often left unsaid that they were considering only nonabsorbing spheres. The last major problem associated with the Shifrin-Perelman group's work was that of inconsistent notation. For example, in the 18 papers I surveyed,  $\tau$  appeared in nine different forms. Although the aforementioned items definitely affected the readability of their collective works, I must say in defense of the Shifrin-Perelman group that the content of their papers still merits attention.

With the aid of Mellin's transformation, Shifrin and Raskin (1961) were the first to substitute  $Q_{\text{ext}}^{\text{AD}}$  into (27) and invert 1. to get  $n(a)$ . When they used anomalous diffraction, the method was termed the transparency method; when they performed a similar inversion in which  $Q_{\text{ext}}$  was derived from the RGD approximation, it was termed the indicatrix method. In the first study, small measurement errors in  $\tau(\lambda)$  lead to large errors in the solution; Shifrin and Perelman (1963a) partially solved this problem. Next, Shifrin and Perelman (1963b) performed a mathematical test. The multispectral extinction was calculated using a  $\gamma$  size distribution; then, this turbidity "data" was used to invert (27). The  $\gamma$ -distribution was reproduced rather well.

Similar tests were later performed for a power-law distribution (Perelman and Shifrin 1968), a  $\beta$ -distribution (Perelman and Shifrin 1969), and a logarithmic distribution (Bakhtiyarov et al. 1966). The latter test was slightly different in that exact Mie values were used for the direct calculation of the "data,"  $\tau(\lambda)$ . Additionally, Bakhtiyarov et al. (1966) finally made mention of the fact that using anomalous diffraction introduces some error, although they claimed it was negligible. Quantitative error analysis was needed but did not come until Shifrin et al. (1969c). In this study, a size distribution was assumed and  $m$  varied. The error arising from using  $Q_{\text{ext}}^{\text{AD}}$  instead of the exact value was 3, 14, 18, and 20% for  $n = 1, 1.1, 1.3, \text{ and } 1.5$ , respectively. To return to the early work, in Shifrin and Perelman (1963c), the effect of various assumptions on the experimental data was analyzed. Also, they showed how to use either graphic or tabular presentations of  $\tau(\lambda)$  to invert (27); improvements were offered in Shifrin et al. (1969b). Shifrin and Perelman (1964a) continued the previous analysis, but this time only for tabular data presentation; also in this paper, qualitative estimates were given of the effect on the determination of  $n(a)$  of errors in the measurement of  $\tau(\lambda)$ . In a jump back to their earlier work, Shifrin and Perelman (1964b) provided a compilation of the first three papers of the group: Shifrin and Raskin (1961) and Shifrin and Perelman (1963a, 1963b). Later that year, Shifrin and Perelman (1964c) discussed the effect of an almost monodisperse  $\gamma$ -distribution on the inversion of (27); additionally, they concluded that although measurements of  $\tau$  were needed at all wavelengths mathematically, 10-20 measurements over a broad wavelength spectrum

would suffice. In one of their better works, Shifrin and Perelman (1965) made a quantitative analysis of the effect of measurement errors of  $\tau$  on the calculation of  $n(a)$ . They found that  $\tau$  had to be measured with an accuracy of 1-2%. Even though the mathematical tests of a  $\gamma$ -distribution had been done, experimental verification of the validity of the inversion was lacking until Shifrin et al. (1966) provided it. The particle spectra derived from the inversion of (27) and from electron micrograph measurements were compared and reasonable agreement was found. The best paper to start with if interested in Shifrin and Perelman's inversion method is theirs of 1966. It is basically a review of their work up to this date. Next, Perelman (1967a) improved the inversion to give better agreement between the transparency and indicatrix methods in the region of small phase shifts. Perelman claimed that anomalous diffraction was valid for  $0 < |m-1| < 1$  whereas the RGD approximation was only valid for  $|m-1| \ll 1$ . While anomalous diffraction can be used for  $m \approx 2$ , it is certainly not a very good approximation there; Perelman's claim should not have been made without qualification. Perelman (1967b) departed from a more physical viewpoint to give a thorough mathematical analysis of the inversion of first kind Fredholm integral relations; this paper is a good source of information on these functions. The only paper of the Shifrin-Perelman group to consider absorbing spheres was that of Perelman and Punina (1969); unfortunately, this paper was available only in German, so I can provide no more information than that given in the abstract. A paper from this group which I recommend avoiding is that of Shifrin et al. (1969a). I am left with the impression that this paper was never proofread. For instance,

even the title has a misprint; the word "Special" appeared where the word "Spectral" should have. There are considerably more errors of this sort and worse throughout the paper, and I do not know whether to place the blame on the authors or the translator. Either way, I see no reason why we should try to decipher it. After a break of 10 years, Shifrin et al. (1979) offered an improved inversion method in which the multispectral extinction data was approximated by modified Legendre polynomials. To avoid divergence of the solution for the Shifrin-Perelman inversion technique, it is necessary to know the short wavelength limit of  $\tau(\lambda)$ . The new approach of Shifrin et al. allowed for the direct extrapolation of  $\tau(\lambda)$  to short wavelengths; in all prior works, it had to be extrapolated separately. In the last papers of the series, Perelman and Shifrin (1979, 1980) finally allowed  $m(\lambda)$  to vary as it should have all along. For their inversion,  $\tau$  must be measured over a broad wavelength spectrum; to assume  $m(\lambda)$  is constant over this entire spectrum is foolish. The improvement was welcome and necessary but long in coming.

Next we consider the Box-McKellar group. I found considerable improvement in the clarity of their approach over that of the Shifrin-Perelman group. The inversion of (27) under the Box-McKellar scheme is dependent on the knowledge of the multispectral extinction and of the zeroth and second moments of the size distribution; physically, these moments are  $N$ , the number of particles per unit volume, and  $\bar{G}$ , the total geometric cross section per unit volume. Details on extracting the two moments from the data were given in Box and McKellar (1976). The actual application of the moments to the inversion of (27) was given

in Box and McKellar (1978b). Their inversion was valid if  $Q_{\text{ext}}^{\text{AD}}$  was substituted for the exact value in the turbidity equation and if  $n(a)$  vanished faster than  $a^\epsilon$  as  $a \rightarrow 0$  for some positive  $\epsilon$ ; this latter requirement is almost always met in practice. Almost simultaneously with Box and McKellar, Fymat (1978a) introduced his own technique for the inversion of (27). Box and McKellar (1979) compared their and Fymat's method and found Fymat's approach to be a more general method than their own. In a further comparison, Box and McKellar (1981) illustrated how their, Fymat's, and Shifrin and Perelman's inversion methods were all related. They also showed that the Shifrin-Perelman technique was the most susceptible to errors. Also in this paper, a new inversion was introduced, although a discussion of its merits were left for an as yet unpublished work. In the conclusion of their 1981 work, Box and McKellar argued as to the value of analytic inversion methods based on anomalous diffraction; they cited Walters (1980) as having claimed to use Shifrin and Perelman's inversion scheme "apparently with some success." However, to quote Walters, "[Shifrin and Perelman's method] must be regarded as being of little value for this type of application." Walters was comparing the size distribution predictions of three inversion methods with experimentally measured size distributions of fogs formed in supersonic stream flows. Besides Shifrin and Perelman's method, he considered an empirical approach and a matrix inversion method. Please note that equation (10) of Walters, which gives  $Q_{\text{ext}}^{\text{AD}}$  for nonabsorbing spheres, is completely wrong; see Table 1 for the correct expression. We cannot conclude that Box and McKellar's inversion scheme is as poor in application; however, Box and

McKellar's optimistic interpretation of Walters' (1980) conclusions makes me wary of any of their claims. The last paper of this group is an outstanding one by Viera and Box (1985). I have already quoted some of their introduction at the beginning of this section. In this paper, an analytic eigenfunction theory was used for the inversion of (27), and to fully exploit the analyticity,  $Q_{\text{ext}}^{\text{AD}}$  was used instead of the exact Mie value. Tests were performed to find the effects of certain assumed knowledge of the solution on the ill-posedness of the problem. The conclusions they reached on what the important factors were should be of interest to those attempting remote sensing experiments in which data inversion must be performed.

Finally, we consider the work of the Fymat group. As mentioned earlier, Fymat (1978a) developed his inversion technique at nearly the same time as Box and McKellar (1978b). Whereas the Box-McKellar approach required a knowledge of the two moments  $N$  and  $\bar{G}$ , Fymat (1978b) showed that his method required only a knowledge of  $\bar{G}$ . Fymat and Smith (1979) continued to expound the virtues of Fymat's method. Since it requires less information than the Box-McKellar method, Fymat's method is simpler than that of the former. Box and McKellar (1978b) concurred with this evaluation. Fymat and Smith gave a nice, concise listing of the conditions necessary for the validity of both the Fymat (1978a) and the Box and McKellar (1978b) inversion techniques. Fymat and Smith noted that equation (10) of Fymat (1978a) was invalid because the integral diverges; the results were unaffected however.

The remainder of this section is devoted to three papers not associated with the previous groups' works. I have already covered

Walters (1980) under the Box-McKellar review. The other two papers are Smith (1982) and Klett (1984). Smith (1982) generalized Fymat's (1978a) inversion technique to allow for the variation of the complex refractive index with wavelength. He used van de Hulst's (1957, p. 179) expression for  $Q_{\text{ext}}^{\text{AD}}$  for absorbing spheres as the kernel of (27). Smith's paper is nicely presented and mathematically complete. Klett (1984) was not aware of Smith's (1982) paper for he cited Perelman and Punina (1969) as the only paper prior to his to consider absorbing spheres for the inversion of (27). Klett, like Smith and Perelman and Punina, used van de Hulst's (1957, p. 179) equation for  $Q_{\text{ext}}^{\text{AD}}$  for absorbing spheres. He gave the expression in his equation (6), but it is given incorrectly. The last term of his equation (6) should contain the factor  $(\cos \beta / \rho)$  squared, not to the first power. Klett otherwise has an excellent paper here. He was the first to really address the practicality of the various inversion methods based on anomalous diffraction. Klett developed a new inversion technique that may be as good or better than all previous methods. He empirically adjusted  $Q_{\text{ext}}^{\text{AD}}$  to give better agreement with the Mie theory before he used it as the kernel of the turbidity equation. Although Klett's inversion scheme may be best, we must wait for conclusive experimental verification of all of the analytic inversion methods based on anomalous diffraction before we can make such a determination.

### 1.3.2 Right Circular Cylinders and Discs

The infinite right circular cylinder is another particle shape for which an exact calculation of the light scattering can be made, yet an infinite cylinder is a physically unrealistic particle. What we

actually wish to consider is a cylinder with an axial ratio (length:width) so large that end effects can be ignored. Bohren and Huffman (1983, p. 211) determined that in the limit of Fraunhofer diffraction, a cylinder could be considered essentially infinite if the axial ratio was greater than 10:1. Since van de Hulst (1957, Ch. 11) developed his approximation from a consideration of Fraunhofer diffraction, I will assume that the same axial ratio applies to anomalous diffraction. Also in this section, I will discuss the thin disc. Although no exact theory applies, a disc is, after all, just a short cylinder.

Unlike the sphere, the cylinder has shape anisotropy; consequently, the optical efficiencies are polarization dependent in the exact theory. Since anomalous diffraction is a scalar theory, however, no polarization dependency is shown. Also because of the cylinder's shape anisotropy, the angle of orientation becomes an important parameter. Even with this additional parameter, we will find that anomalous diffraction works quite well for the cylinder and yet is still simple.

#### 1.3.2.1 Single Cylinders and Discs

Van de Hulst (1957, p. 313) obtained a closed-form solution for  $Q_{\text{ext}}^{\text{AD}}$  of an infinite, nonabsorbing cylinder at normal incidence. Little discussion was offered, and the expression did not reappear until Kerker (1969, p. 290) cited it in his review of anomalous diffraction. Later that same year, Bryant and Latimer (1969) generalized van de Hulst's work by giving  $Q_{\text{ext}}^{\text{AD}}$  and  $Q_{\text{abs}}^{\text{AD}}$  for arbitrarily oriented, absorbing infinite cylinders; they also gave the same quantities for a thin disc. A closed-form expression for  $Q_{\text{ext}}^{\text{AD}}$  or  $Q_{\text{abs}}^{\text{AD}}$  was not yet offered for the



cylinder, but such expressions were given for the disc (see Table 2). In the overview, I noted that  $Q_{\text{ext}}^{\text{AD}}$  approaches the correct asymptotic value of two as  $x \rightarrow \infty$  for many particle shapes, the nonabsorbing disc is not such a shape. To the incoming light, the face of an infinite disc would appear as a slab; the phase shift through all portions would be the same. For the case of no absorption,  $Q_{\text{ext}}^{\text{AD}}$  for a disc takes the form of an undamped, oscillating function (see Table 2); as  $x \rightarrow \infty$ ,  $Q_{\text{ext}}^{\text{AD}}$  can assume any value between two and four.

In 1970, closed-form expressions for  $Q_{\text{ext}}^{\text{AD}}$  and  $Q_{\text{abs}}^{\text{AD}}$  for the absorbing, infinite cylinder at arbitrary incidence were finally given by Cross and Latimer. The angle of incidence was defined by the normal to the cylinder axis and the incident direction. Cross and Latimer noted that at very oblique incidence, refraction effects could not be ignored, so they offered an empirical factor to correct for these effects. Cross and Latimer's paper was outstanding in its straightforwardness and simplicity. Their paper was quite a contrast to Stephens' (1984). Stephens apparently unaware of the previous results of Cross and Latimer, obtained his own closed-form expressions for  $Q_{\text{ext}}^{\text{AD}}$  and  $Q_{\text{abs}}^{\text{AD}}$  for the arbitrarily oriented, absorbing, infinite cylinder. In Stephens' paper, the angle of incidence was defined by the cylinder axis and the incident direction. Stephens' expressions for  $Q_{\text{ext}}^{\text{AD}}$  and  $Q_{\text{abs}}^{\text{AD}}$  appear at first sight to be quite different from those of Cross and Latimer, but I have shown that the expressions are equivalent (see Table 3). Stephens' relation for  $Q_{\text{abs}}^{\text{AD}}$  was actually not different at all, rather it suffered from the following typographical error: the  $L_1$  in his equation (21) should have been an  $L$ . Stephens' paper has many other

errors, some typographical, some not. Stephens began his paper rather well by giving the exact theory in detail. He went on to find the expressions for  $Q_{\text{ext}}^{\text{AD}}$  and  $Q_{\text{abs}}^{\text{AD}}$  and used the former to find  $\bar{Q}_{\text{ext}}$  for two cases: (i) a monodispersion of randomly oriented, nonabsorbing cylinders, and (ii) a polydispersion of oriented, nonabsorbing cylinders. For the latter case, Stephens' equations (23), (24), (26), and (27), giving respectively  $\bar{G}$ ,  $\tau$ ,  $a_{\text{eff}}$ , the effect radius of the distribution, and  $V_{\text{eff}}$ , the effective variance of the distribution, are all incorrect. These four equations, as they stand, are valid only for spheres, not cylinders. Assuming normal incidence, the factor  $\pi a^2$  in each equation should be replaced by the factor  $2aL$ , where  $L$  is the length of the cylinder. In his equation (26), the factor  $\pi a^3$  should be replaced by the factor  $\pi a^2 L$ . Fortunately, the graphs resulting from these equations were unaffected by the errors. I think Stephens' paper illustrates the importance of accurate proofreading very well. In addition to the aforementioned errors, Stephens also badly misinterpreted the meaning of  $n'$ ; since I discussed this previously, I will not repeat it here. Stephens has assured me that an errata will be forthcoming.

As with spheres, papers comparing the predictions of anomalous diffraction to those of the exact theory can also be found for cylinders. The first, for real  $m$  only, was that of Sharma et al. (1981). They compared the anomalous diffraction, RGD, Eikonal, and first-order corrected Eikonal (FCE) approximations predictions of the forward scattered light intensity with those of the exact theory for  $\lambda = 0.6328 \mu\text{m}$ ,  $1.05 \leq n \leq 1.5$ , and  $0.2 \leq x \leq 25$ . The first-order

correction to the Eikonal approximation was not elaborated on; it makes the Eikonal approximation much more complex, but the results are considerably improved. Whereas no similar study was done for spheres with complex  $m$ , such a study was performed for cylinders with complex  $m$  by Sharma and Somerford (1983). The same approximations as in Sharma et al. (1981) were compared in the same way for  $1.05 \leq n \leq 1.15$ ,  $10^{-3} \leq n \leq 1$ ,  $1 \leq x \leq 20$ , and  $\lambda = 0.6328 \mu\text{m}$ . I have already cited the usefulness of such papers and will not do so again. The final comparison paper, similar to the previous two, is that of Sharma and Somerford (1982). Like the previous two papers, the same approximations were compared with the exact theory. Unlike the previous two papers, the  $0^\circ \leq \theta \leq 60^\circ$  scattered light intensity was used for the comparison. The incident light was assumed normal to the cylinder axis; the scattered light intensity in the plane of the normal was calculated. The authors claimed that anomalous diffraction was a poor approximation to the exact theory for all trials, but their figures indicated that it worked fairly well for  $\theta < 30^\circ$  and  $n \leq 1.5$ . Part of the reason for the poor predictions of anomalous diffraction may lie in the expression that Sharma and Somerford used for their anomalous diffraction calculations. Sharma and Somerford purported to have used van de Hulst's (1957, p. 184) approach to getting  $S(\theta)$  from  $S(0)$ , yet I can in no way determine how. Their  $S(\theta)$  agrees with my equation (16) for  $\phi = 0^\circ$  except that where I have the factor  $\exp(-ik\xi\theta)$  under my integral, they have the factor  $\cos(ik\xi\theta) = \text{Re}\{\exp(-ik\xi\theta)\}$ . My more general expression reduces to van de Hulst's for spheres and is in agreement with Meeten

(1982b); consequently, I suspect Sharma and Somerford's expression to be in error.

#### 1.3.2.2 Monodispersions

Only Bryant and Latimer (1969), Champion et al. (1978), and Stephens (1984) considered cylindrical monodispersions. I have said all that I will about the latter paper. Bryant and Latimer gave a nice synopsis of methods for calculating the turbidity of randomly oriented cylinders and discs. Bryant and Latimer noted that a thin disc, for example, may present a dimension to the incident beam which is in violation of the condition for the applicability of anomalous diffraction; however, they concluded that few enough particles would be oriented at such extremes so as not to affect the results significantly. The paper by Champion et al. (1978) was previously discussed in section 1.3.1.2, and my comments can be found there. They derived expressions for the refractive index increment of colloidal spheres and oriented discs in the Rayleigh, RGD, and anomalous diffraction approximations.

#### 1.3.2.3 Polydispersions

Stephens (1984) is the only source here. He considered only aligned cylinders. Because of the many errors in Stephens' paper, I recommend that it be used with extreme caution.

#### 1.3.2.4 Biological Particles

Bryant et al. (1969a) is the only source here. They modeled E. Coli cells as infinite cylinders with good results. For further details, consult section 1.3.1.4 where this paper was reviewed.

#### 1.3.3 Cubes, Square Plates, Hexagonal Plates and Octagonal Plates

Anomalous diffraction is of greater utility for cubes and thin square, hexagonal, or octagonal plates than for spheres and cylinders

because no exact solutions exists for these particle shapes. Yet crystals of these shapes are often encountered in nature, the hexagonal plate of ice being a familiar example. The RGD approximation can be applied to these shapes but is not as accurate as anomalous diffraction in the size range  $1 \leq x \leq 20$ .

#### 1.3.3.1 Single Particles

The first paper of this section and the only one to consider cubes was that of Napper (1967). He derived  $Q_{\text{ext}}^{\text{AD}}$  assuming real  $m$  for three simple cube orientations: face, corner, and edge incidence. Table 4 gives the expressions. The relation for  $Q_{\text{ext}}^{\text{AD}}$  of a nonabsorbing cube at face incidence is the same as that for a nonabsorbing disc at face incidence; therefore, the cube is another particle shape for which  $Q_{\text{ext}}^{\text{AD}}$  does not approach its correct limit as  $x \rightarrow \infty$ . Napper made an admittedly crude attempt to model a monodispersion of randomly oriented cubes by assuming that the probabilities of face, corner, and edge incidence were 3:6:4, respectively. Napper's paper was clear and concise; I think he demonstrated the need for approximate theories rather nicely. Kerker (1969, p. 127) gave a review of Napper's work.

Next, Champion et al. (1979a) used anomalous diffraction to successfully predict experimentally observed transmission changes in shear-flow oriented monodispersions of kaolinite crystals. The transmission changes were induced by varying the velocity gradient of the orienting medium, the particle size, the wavelength, or the crystal concentration. Kaolinite crystals are hexagonal plates but are rarely found in perfect form, thus square and octagonal plates were considered as models of chipped crystals. The crystals were assumed to be thin and

nonabsorbing; a 10:1 axial ratio was used in all calculations. Champion et al. assumed that the light traversed the thinnest dimension of the crystals; they provided expressions for  $C_{\text{ext}}^{\text{AD}}$  for all three crystal shapes at various orientations. Champion et al., in contrast to Napper (1967), were difficult to follow and some of the notation was poor.

#### 1.3.3.2 Monodispersions

It is evident from the previous section that Napper (1967) and Champion et al. (1979a) applied their approximations to monodispersions; however, I will not repeat my comments here. The only other paper to consider is that of Meeten (1979). Meeten used anomalous diffraction to derive an expression for the optical anisotropy parameter. For an optically anisotropic particle of optic axes,  $a$ ,  $b$ , and  $c$ , with refractive indices of  $m_a$ ,  $m_b$ , and  $m_c = m_b$ , respectively, the optical anisotropy parameter is proportional to  $(m_a - m_b)$ . A previous formulation of the optical anisotropy parameter, which was derived from a dipole approach, predicted no size dependence for the parameter, yet size dependence was observed experimentally. Meeten found that his approach, using anomalous diffraction, gave a satisfactory explanation of the experimentally observed size dependence of the optical anisotropy parameter for weakly birefringent kaolinite crystals. Meeten considered the same crystal shapes as Champion et al. (1979a), i.e., the square, hexagonal, and octagonal plates. Immediately following equation (18) of Meeten, there is a misprint which I feel must be corrected. In a single sentence, Meeten claimed that the size parameter  $x$  was dimensionless then gave it as  $x = \frac{1}{2}k$  which is dimensional. Meeten must have intended  $x = \frac{1}{2}kt$  where  $t$  is the thickness of the particle over which the light is

transmitted. The reason I found the error so troubling was that two graphs soon followed in Meeten's paper in which  $x$  was a coordinate.

#### 1.3.4 Spheroids

The spheroid, an ellipsoid of revolution, has become an increasingly popular shape with researchers over the past two decades. Only recently has an exact solution for light scattering by an ellipsoid become available (Asano and Yamamoto 1975). The exact solution is rather cumbersome to use in practice, so the anomalous diffraction expressions for the optical efficiencies are still welcome. We will assume the spheroids to have axes of radii  $a$ ,  $a$ , and  $b$ ; the axial ratio is given by  $v = b/a$ . For the oblate spheroid,  $v < 1$ ; for the prolate spheroid,  $v > 1$ . The popularity of the spheroid is due to the fact that it can be used to approximate other particle shapes. For instance, a highly oblate spheroid is an excellent model of a disc while a highly prolate spheroid is an excellent model of a cylinder. On the other hand, as the axial ratio approaches unity, the spheroid reduces to a sphere. The deviation of the axial ratio from unity is usually referred to as the asphericity.

##### 1.3.4.1 Single Spheroids

The first paper of this section is that of Bryant and Latimer (1969). This is an excellent paper on anomalous diffraction in general, and I have already cited it in the sphere and cylinder sections. Bryant and Latimer's approach to obtaining  $Q_{\text{ext}}^{\text{AD}}$  and  $Q_{\text{abs}}^{\text{AD}}$  of the spheroid was to model it as a sphere with a modified phase shift; see Table 5 for the results. They provided superb graphs illustrating the effect of particle shape (sphere, disc, cylinder, and cube) on  $Q_{\text{ext}}^{\text{AD}}$  and  $Q_{\text{abs}}^{\text{AD}}$ .

Bryant and Latimer also gave a fine review of ways to calculate  $\bar{Q}_{\text{ext}}$  and  $\bar{Q}_{\text{abs}}$  for monodispersions of various (cylinders, discs, and spheroids) randomly oriented particles. Furthermore, they showed that for small asphericity ( $v \approx 2$ ), a randomly oriented monodispersion of spheroids could be approximated very well by a monodispersion of spheres of equal volume. One point I disliked about their graphs was that  $m$  was not usually given, thus the graphs seemed untied to reality. Latimer (1975a) developed an improved, yet considerably more complex hybrid method to predict light scattering by spheroids; the hybrid was based on both anomalous diffraction and Mie theory. First, anomalous diffraction principles were applied to a spheroid of given size, shape, orientation, and refractive index, and the results were used to define an equivalent sphere; subsequently, the exact Mie theory was used to calculate the scattering of this equivalent sphere. In the method Latimer denoted AM-I, the radius of the spheroid was redefined; in the method he denoted AM-II the refractive index of the spheroid was redefined. Latimer used the RGD approximation in an identical way to get the similar methods RM-I and RM-II. Latimer's paper was often vague; at times it was not clear which method or which particle (equivalent sphere or spheroid?) he was discussing. For a monodispersion of randomly oriented spheroids, Latimer presented graphs of scattered intensity versus angle in which he compared his various methods. I did not see the value in this since he had not yet determined how well any of the approximations compared with experimental observations (the exact solution for spheroids was not available at this date). In Latimer and Barber (1978), the predictions



of scattered light intensity of Latimer's (1975a) methods were compared to the same predictions of the extended boundary condition method (EBCM) of Barber and Yeh (1975). All calculations were for real  $m$  only. The EBCM solves Maxwell's equations numerically for spheroids and other particle shapes. All of the methods were in good agreement except for AM-I. Regardless, Latimer and Barber felt compelled to include it in their already overcrowded graphs. In another follow-up to Latimer (1975a), Latimer et al. (1978) used the former's methods AM-II, RM-I, and RM-II to compute and compare scattered light intensities for several spheroid axial ratios and at different orientations. Latimer et al. presented excellent polar plots of the angular scattering intensity for the various spheroids considered. Since the exact Mie theory was used, angular intensities could be calculated at all angles; however, since the equivalent spheres were derived from an anomalous diffraction consideration in the AM-II method, I question the validity of large angle scattering calculations for AM-II. Latimer et al. went on to give a nice discussion of various particle-sizing apparatus and techniques; they determined that for spheroids, the shape and orientation would most affect the results; the refractive index effects would be secondary. Latimer informed me that equations (A2) and (A3) of Latimer et al. (1978) were incorrect; they should be corrected as follows (in their notation): (i) in (A2), the  $\cos(\theta/2)$  in the first term and the  $\sin(\theta/2)$  in the second term should be interchanged; (ii) in (A3), the  $\cos \psi$  in the second term should be a  $\cos \omega$ . Next, Latimer (1980) compared his approximate methods' (AM-II and RM-I) predictions of  $\bar{Q}_{\text{ext}}$  for a monodispersion of randomly oriented spheroids with published values of

the same derived from the exact theory for  $m = 1.33$  and  $m = 1.33 - 0.05i$  (Asano and Sato 1980). The agreement was even better than Latimer expected; even the worst agreement, for very oblate spheroids, was within 10% of the exact values.

Another method for predicting light scattering by spheroids was discussed in a 1982 paper by Ravey and Mazeron. The method was termed the physical optics approximation (POA) in order to distinguish it from the simpler approach of geometric optics. In the POA, Maxwell's equations are integrated over the surface of the scatterer; since the fields at all points on the scatterer are not known in general, they must be approximated. In the approximation, it is assumed that the fields at any point on the surface can be given by Fresnel's equations evaluated on a plane tangent to the point. In this paper, Ravey and Mazeron presented the POA and noted how it could be applied to part of the domain of anomalous diffraction; for the POA,  $2x|m-1| \gg 1$  is required. Erroneously, Ravey and Mazeron claimed that for anomalous diffraction, both  $n$  and  $n'$  had to be near unity;  $n' \ll 1$  is the correct requirement. In a follow-up study, Ravey and Mazeron (1983) compared various light scattering predictions of the POA with those of the Mie theory, the RGD approximation, anomalous diffraction, and Fraunhofer diffraction for spheres and with those of the exact method, EBCM, the RGD approximation, and anomalous diffraction for spheroids. Real and complex  $m$  were considered. Ravey and Mazeron presented their results in easy-to-read graphs. For its complexity, the POA does not seem to work as well as anomalous diffraction for spheres; it is better for certain spheroid orientations, however. The anomalous diffraction computations

for spheroids were similar to the simple method of Bryant and Latimer (1969); it would have been interesting to see the POA compared to Latimer's (1975a) methods for spheroids. Ravey and Mazon are, like many others, guilty of misinterpreting  $n'$ . They called  $n' = 0.01$  "small" absorption, yet gave no indication of wavelength. I suspect from their content that Ravey and Mazon were assuming wavelengths of the order of visible light, hence  $n' = 0.01$  would imply "very strong" absorption. In a continuance of the previous work, Ravey (1985) explored the dependence on real refractive index of the first extrema in the angular light scattering pattern of spheres and spheroids. He compared the predictions of the POA, the RGD approximation, Fraunhofer diffraction, and anomalous diffraction. As Ravey and Mazon (1983) had done, Ravey presented his results in excellently prepared graphs. Ravey's study showed how good anomalous diffraction could be considering its simplicity.

#### 1.3.4.2 Monodispersions

Bryant and Latimer (1969) and Latimer (1975a, 1980) all considered monodispersions. For details on these papers, consult the previous section. The only other papers to consider in this section are those of Khlebtsov and Shchegolev (1977), Khlebtsov et al. (1978a), and Meeten (1980c, 1982a).

Khlebtsov and Shchegolev (1977) and Khlebtsov et al. (1978a) are papers very much like those of Box and McKellar (1978a) and Fymat and Mease (1978) in that while the study of the inverse problem of light scattering was their ultimate goal, the direct problem was considered first so as to gain insight into the dependencies of the important

parameters; consult section 1.3.1.3 for further details. Khlebtsov and Shchegolev (1977) used anomalous diffraction expressions for  $Q_{\text{ext}}$  to calculate  $\bar{Q}_{\text{ext}}$ ,  $\tau/N$ ,  $w$ , and  $s$ , the structure factor, for a monodisperse system of randomly oriented prolate spheroids. Equation (26) of this thesis gave  $w$ ; it is related to  $s$  by

$$s = w \left( \frac{\partial Q_{\text{ext}}}{\partial \phi} \right)^{-1} \quad (28)$$

Note that for this study,  $Q_{\text{ext}}$  would be replaced with  $\bar{Q}_{\text{ext}}$  in (26) and (28). The dependence of the four parameters on real  $m$ ,  $x$ , and  $\phi$  was desired for future research on inversion methods for spheroids; for further information on these inversion methods, consult all of section 1.3.4.4. Khlebtsov et al. (1978a) conducted a completely analogous study for randomly oriented oblate spheroids. Additionally, however, they calculated the same four parameters using the RGD approximation. Both Khlebtsov and Shchegolev (1977) and Khlebtsov et al. (1978a) provided excellent tables illustrating the dependence of  $\bar{Q}_{\text{ext}}$  on  $w$  and  $\phi$  for various axial ratios.

Meeten (1980c) is a good, simple paper. In it, the Rayleigh, RGD, and anomalous diffraction approximations were used to find the effect of particle shape on the refractive index of a colloidal dispersion. The dispersion was modeled as a collection of randomly oriented, nonabsorbing spheroids; the effect of asphericity on the refractive index of the dispersions was predicted to be large by all three approximations. Interestingly, the expressions Meeten derived from all of the approximations approached the same limit as  $(m-1) \rightarrow 0$  and  $x \rightarrow 0$ .

Meeten (1982a) derived integral expressions for the linear birefringence and linear dichroism of a colloidal dispersion of nearly aligned, optically anisotropic, nonabsorbing spheroids. This paper continues the work begun in Meeten's 1980a and 1980b papers; since the application of anomalous diffraction is essentially the same here, I refer the interested reader to my reviews of the 1980a and 1980b papers in section 1.3.1.2.

#### 1.3.4.3 Biological Particles

Many biological cells could be modeled as being spheroidal; however, the literature on anomalous diffraction in which this is done is scarce. The first paper to appear along these lines was that of Bryant et al. (1969a). They used anomalous diffraction applied to a spheroid to model scattering by yeast cells and spinach chloroplasts. Bryant et al.'s theoretical predictions were in good agreement with experimentally determined light intensities from both of these particles. For further details on this paper, I refer the reader to section 1.3.1.4. Later, Latimer (1975b) used the AM-II method of his 1975a paper to try to theoretically predict the experimentally observed changes in extinction that arose from structural changes in blood platelets. The actual structural change is that the originally disc-like platelets become nearly spherical upon activation by certain compounds. The spheroid then was a useful model since it could be used to represent both extremes of the platelet shape. Latimer's theoretical predictions were in agreement with experimental observations, thus the value of his simple model became evident. Lastly, Ravey (1985) explored the evolution of the first extrema of the angular scattering intensity

as the refractive index was changed. He considered spheres and spheroids and assumed both were nonabsorbing. I have already reviewed this paper under the single spheroid section, and my comments will not be repeated. I included this paper here because it arose out of Ravey's interest in the determination of blood cell size from small angle light scattering measurements. Blood cells are nearly spheroidal in shape.

#### 1.3.4.4 Inversion Techniques

The papers in the following section on monodispersions are the last of this literature review. Unlike for spheres, no studies were done on analytic inversion techniques for spheroidal polydispersions.

##### 1.3.4.4.1 Monodispersions

Shchegolev and Klenin (1970, 1971), both of which were reviewed under section 1.3.1.5.1, showed that for spheres, measurements of  $\tau(\lambda)$  over a narrow wavelength spectrum could be used to find the size, concentration, and refractive index of the spheres if the wave exponent and structure factor were also known. For a spheroidal monodispersion, these parameters (size, concentration, refractive index) can also be calculated, but they apply to a sphere of equal volume. Shchegolev et al. (1977) used mathematical tests to find the error incurred by considering such equivalent spheres. The direct calculations of  $\tau/N$ ,  $w$ , and  $s$  for prolate spheroids from Shchegolev and Klenin (1977) were used as the input "data"; then, the size, concentration, and refractive index of equivalent spheres were calculated from this "data." I do not think this was very good test; since the "experimental data" arose from the anomalous diffraction approximation, some real information was necessarily lost. The actual error is probably somewhat higher than

Shchegolev et al. reported. As expected, use of the equivalent sphere method gave best agreement for small asphericity. A similar test was performed in which the RGD approximation was used. Khlebtsov et al. (1978b) performed an identical analysis to that of Shchegolev et al. (1977) except that they considered oblate spheroids. The direct calculations of  $\tau/N$ ,  $w$ , and  $s$  for oblate spheroids from Khlebtsov et al. (1978a) were used as the input "data." The final paper of this literature review is that of Khlebtsov et al. (1978c). They showed, using both the RGD and anomalous diffraction approximations, that the minor semi-axes and weight concentration of highly aspheric, randomly oriented spheroids could be calculated from a knowledge of the wave exponent. The spheroid could be highly oblate or prolate, and the predicted values could be very accurate depending on the values of the wave exponent and axial ratio.

Table 1. The anomalous diffraction expressions for the extinction and absorption efficiencies of a sphere of radius  $a$ . In this table,  $\phi = 2x(m-1)$ ,  $\tan \beta = n'/(n-1)$ ,  $H$  is the Struve function,  $y$  is the spherical Bessel function of the second kind,  $J$  and  $j$  are the Bessel and spherical Bessel functions of the first kind, respectively, and  $F$  is the hypergeometric function.

Function	Expression	Source
(1) (Real m)		
$Q_{\text{ext}} =$	$2 - \frac{4 \sin \phi}{\phi} + \frac{4(1 - \cos \phi)}{\phi^2}$	van de Hulst (1957)
$=$	$2\phi \int_0^1 (1 - t^2) \sin(\phi t) dt$	Shifrin and Perelman (1979)
$=$	$4\left(\frac{\pi}{2\phi}\right)^{1/2} H_{3/2}(\phi)$	Box and McKellar (1976)
$=$	$2\left(1 + \frac{2}{\phi}\right) + 4y_1(\phi)$	Fymat (1978a)
$=$	$2\left(1 + \frac{2}{\phi}\right) + 4j_{-2}(\phi)$	Fymat (1978a)
$=$	$2\left(1 + \frac{2}{\phi}\right) + 2\left(\frac{2\pi}{\phi}\right)^{1/2} J_{-3/2}(\phi)$	Fymat (1978a)
$=$	$\frac{1}{2} \phi^2 F(1; 3, 3/2; -\frac{1}{4} \phi^2)$	Fymat (1978a)



Table 1. (Continued)

Function	Expression	Source
$Q_{\text{ext}} =$	$2\left(1 + \frac{2}{\phi^2}\right) + 4 \frac{d}{d\phi} \left(\frac{\cos \phi}{\phi}\right)$	Fymat and Smith (1979)
$=$	$2 + 4 \frac{d}{d\phi} \left(\frac{\cos \phi - 1}{\phi}\right)$	Fymat and Smith (1979)
(2) (Complex m)		
$Q_{\text{ext}} =$	$2 - 4 \exp(-\phi \tan \beta) \left(\frac{\cos \beta}{\phi}\right) \left\{ \sin(\phi - \beta) + \left(\frac{\cos \beta}{\phi}\right) \cos(\phi - 2\beta) \right\}$ $+ 4 \left(\frac{\cos \beta}{\phi}\right)^2 \cos 2\beta$	van de Hulst (1957)
$Q_{\text{abs}} =$	$1 + \frac{\exp(-2\phi \tan \beta)}{\phi \tan \beta} + \frac{\exp(-2\phi \tan \beta) - 1}{2\phi^2 \tan^2 \beta}$	van de Hulst (1957)

Table 2. The anomalous diffraction expressions for the extinction and absorption efficiencies of a disc of thickness  $t$  and radius  $a$  at arbitrary orientation. It is assumed that the thickness  $t$  makes a negligible contribution to the facial area of the disc. In this table,  $\phi = k t_0 (n-1) \sec x$ ,  $x$  is the angle between the incident direction and the normal to the face, and  $\tan \beta = n'/(n-1)$ .

Function	Expression	Source
(1) (Real m)		
$Q_{\text{ext}} =$	$2 - 2 \cos \phi$	Bryant and Latimer (1969)
(2) (Complex m)		
$Q_{\text{ext}} =$	$2 - 2 \exp(-\phi \tan \beta) \cos \phi$	Bryant and Latimer (1969)
$Q_{\text{abs}} =$	$1 - \exp(-2\phi \tan \beta)$	Bryant and Latimer (1969)

Table 3. The anomalous diffraction expressions for the extinction and absorption efficiencies of a cylinder of radius  $a$  at arbitrary orientation. In this table,  $\phi = 2x(m-1)\csc x$ ,  $x$  is the angle between the incident direction and cylinder axis,  $\phi' = \phi(1-i\tan\beta)$ ,  $\tan\beta = n'/(n-1)$ ,  $H$  is the Struve function,  $J$  is the Bessel function,  $L$  is the modified Struve function and  $I$  is the modified Bessel function. Note that  $H_1(\phi') = I_1(i\phi')$  and  $iJ_1(\phi') = -L_1(i\phi')$ .

Function	Expression	Source
(1) (Real m)		
$Q_{\text{ext}} =$	$\pi H_1(\phi)$	Stevens (1984)
(2) (Complex m)		
$Q_{\text{ext}} =$	$\pi \operatorname{Re}\{H_1(\phi') + iJ_1(\phi')\}$	Cross and Latimer (1970)
	$\pi \operatorname{Re}\{I_1(i\phi') - L_1(i\phi')\}$	Stephens (1984)
$Q_{\text{abs}} =$	$\pi/2 [I_1(4xn'\csc x) - L_1(4xn'\csc x)]$	Cross and Latimer (1970) Stephens (1984)

Table 4. The anomalous diffraction expressions for the extinction efficiency of a nonabsorbing cube of side  $\ell$  at face, corner and edge orientation. In this table,  $\phi = k\ell(m-1)$ . For face incidence, the normal to a face and the incident direction are parallel. For edge incidence, propagation is along a square diagonal. For corner incidence, propagation is along a body diagonal.

<u>Function</u>	<u>Orientation</u>	<u>Expression</u>	<u>Source</u>
$Q_{\text{ext}} =$	Face	$2 - 2 \cos \phi$	Napper (1967)
$Q_{\text{ext}} =$	Edge	$2 - \{(2)^{\frac{1}{2}} \sin [(2)^{\frac{1}{2}} \phi]\} \phi^{-1}$	Napper (1967)
$Q_{\text{ext}} =$	Corner	$2 - 4/3 \{[1 - \cos [(3)^{\frac{1}{2}} \phi]]\} \phi^{-2}$	Napper (1967)

Table 5. The anomalous diffraction expressions for the extinction and absorption efficiencies\* of a spheroid at arbitrary orientation and with arbitrary axial ratio.<sup>2</sup> The axes are assigned the lengths a, a, and b. In this table,  $\phi = 2ka(n-1)[\sin^2 \theta + (a/b)^2 \cos^2 \theta]^{-1/2}$ ,  $\phi' = \phi(1 - i \tan \beta)$ ,  $\tan \beta = n'/(n-1)$ ,  $G(\theta)$  is the geometric area of the spheroid projected onto a plane perpendicular to the incident direction, and  $\theta$  is the angle between the incident direction and the spheroid's symmetry axis.

Function	Expression	Source
(1) (Real m)		
$Q_{\text{ext}} =$	$\frac{2}{G(\theta)} \int G(\theta) [1 - \exp(-i\phi(\theta))] dG$	Bryant and Latimer (1969)
(2) (Complex m)		
$Q_{\text{ext}} =$	$\frac{2}{G(\theta)} \int G(\theta) [1 - \exp(-i\phi'(\theta))] dG$	Bryant and Latimer (1969)
$Q_{\text{abs}} =$	$\frac{2}{G(\theta)} \int G(\theta) [1 - \exp(-2\phi(\theta) \tan \beta)] dG$	Bryant and Latimer (1969)

\* For more accurate, yet more complex expressions of  $Q_{\text{ext}}$  and  $Q_{\text{abs}}$ , see Latimer (1975a).

## Chapter 2

### THEORY

#### 2.1 The Problem

In the usual considerations of diffraction, an arbitrary wave is incident from the  $-z$  direction on certain apertures in an infinite, perfectly conducting thin screen  $S$ . Assuming the apertures to be located in the plane  $z = 0$ , then the field at  $z > 0$  will be in directions other than the incident due to the presence of the apertures. For many purposes, it is sufficient to consider the incident wave to be a scalar wave. If the wavelength of the incident wave is small compared with the dimensions of the aperture, then Kirchhoff's (scalar) mathematical formulation of Huygen's principle can be used to calculate the field at  $z > 0$  which we will call the diffracted field. In order to use Kirchhoff's formula, it is necessary to know the value of both the wave and its gradient over every portion of the plane  $z = 0$ ; however, these values in general are not known, thus approximate values must be used. In the Kirchhoff approximation, the values of the wave and its gradient are assumed to be zero everywhere on  $S$ ; these values in the apertures are assumed to be those of the incident field. Further simplification arises in the calculation of the diffracted field if we assume that the observation point is many wavelengths removed from the apertures, in other words, if we assume we are in the far field; this last assumption confines consideration of diffraction to what is historically referred to as the Fraunhofer zone. In fact, when diffraction is mentioned in the literature, it is usually Fraunhofer diffraction which is meant.

Once the diffracted field arising from the apertures is known, Babinet's principle becomes useful. Babinet's principle relates the diffracted fields of a particular diffracting system to those of its complement. As a simple example, let us consider a screen with a circular aperture of radius  $a$  cut into it; the complementary screen is a disc of radius  $a$ . Babinet's principle tells us that the diffraction patterns of both systems are equivalent, in fact, the diffraction pattern by a perfectly opaque sphere of radius  $a$  is also the same within the limits of the approximation.

Van de Hulst derived his anomalous diffraction approximation from the considerations of the previous two paragraphs, although he generalized them to allow for transmitted light. Since anomalous diffraction was derived from scalar postulates, the polarization state of the incident radiation is not a factor in the calculations of  $Q_{\text{ext}}$ ,  $Q_{\text{abs}}$ , and  $dC_{\text{sca}}/d\Omega$ . In general, however, these efficiencies are functions of the polarization state of the incident beam. An exception is the homogeneous sphere; both  $Q_{\text{ext}}$  and  $Q_{\text{abs}}$  are polarization independent due to the sphere's symmetry. I consider the polarization independence of anomalous diffraction to be its greatest disadvantage. Perhaps this deficiency could be overcome by the application of vector formulations of diffraction to anomalous diffraction; this is the purpose of this thesis and the derivation will follow.

## 2.1 Vector Formulations of Anomalous Diffraction

In the next two sections, anomalous diffraction expressions will be developed from a consideration of both the Kirchhoff and Kirchhoff-Kottler

vector formulations of Huygen's principle. The derivation will proceed analogously with that of section 1.2 except that here I will consider only  $Q_{\text{ext}}$  and  $dC_{\text{sca}}/d\Omega$  for a right circular cylinder; there is no need to complicate matters with exotic particle shapes until the validity of the approach is either proved or disproved. The right circular cylinder is probably the simplest shape-anisotropic particle to consider with an anomalous diffraction approach. The cylinder will be assumed to have a length of  $L$  and a width of  $2a$ .

Only steady state problems will be considered. The time factor of the electric ( $\vec{E}$ ) and magnetic ( $\vec{H}$ ) fields will not be explicitly written, but it will be understood to be  $\exp(-i\omega t)$  where  $\omega$  is the angular frequency and  $t$  is the time. The right-hand Cartesian coordinates  $\xi$ ,  $\eta$  and  $z$  will be used with corresponding unit vectors  $\hat{e}_1$ ,  $\hat{e}_2$  and  $\hat{e}_3$ . I will let the cylinder's long axis lie along the  $\xi$  axis and let the incident beam be from the  $-z$  axis. Since any polarization state can be expressed as some linear combination of two mutually orthogonal polarization states, I will consider the two cases of transverse magnetic (TM) and transverse electric (TE) polarizations. Assuming normal incidence, and designating the incident wave vector as  $\vec{k}_0 = k\hat{e}_3$ , we find the following expressions: (i) for TM polarization, the incident fields are given by

$$\begin{aligned}\vec{E}_0 &= E_0 \hat{e}_1 \exp(ik_0 z) \\ \vec{H}_0 &= H_0 \hat{e}_2 \exp(ik_0 z)\end{aligned}\tag{29}$$

(ii) for TE polarization, the incident fields are given by



$$\vec{E}_0 = -E_0 \hat{e}_2 \exp(ik_0 z) \quad (30)$$

$$\vec{H}_0 = H_0 \hat{e}_1 \exp(ik_0 z)$$

Outside the diffracting system, all space will be considered to be homogeneous and isotropic with a real index of refraction equal to one. With the preceding points in mind, I will begin.

### 2.2.1 Application of the Kirchoff Formula

Jackson (1975, p. 432) provided Kirchoff's vector formulation of Huygen's principle. In this approach, the scalar Kirchoff formula is simply applied to each of the six field components (three each from  $\vec{E}$  and  $\vec{H}$ ).

For the vector case, equation (6) becomes

$$C_{\text{ext}} = \frac{4\pi}{k^2} \text{Re} \{ \vec{S}(0) \cdot \hat{e}_{0E} \} = G Q_{\text{ext}} \quad (31)$$

where  $\vec{S}(0)$  is the vector forward scattering amplitude, and  $\hat{e}_{0E}$  is a unit vector in the direction of polarization of the incident electric vector. Appendix A provides details of the calculation of  $\vec{S}(0)$  from the Kirchoff formula. In analogy with van de Hulst, we will generalize  $\vec{S}(0)$  to include rays transmitted through the cylinder, thus equation (51) becomes

$$\vec{S}(0) = \frac{-k^2}{2\pi} [\hat{e}_3 \times (\hat{e}_3 \times \hat{e}_{0E})] \int_A (1 - e^{-i\Phi}) d\xi d\eta \quad (32)$$

The substitution of  $\hat{e}_1 = \hat{e}_{0E}$  for a TM wave or  $-\hat{e}_2 = \hat{e}_{0E}$  for a TE wave into equations (31) and (32) will give equal values of  $Q_{\text{ext}}$ ; therefore,

the modification of anomalous diffraction with the Kirchoff formulation of vector diffraction still fails to predict a polarization dependent extinction efficiency.

To calculate the differential scattering cross section, we need to add a factor to  $\vec{S}(0)$ . By analogy with equation (16), we get

$$\vec{S}(\theta, \phi) = \frac{-k^2(1+\cos\theta)}{4\pi} [\hat{e}_k \times (\hat{e}_3 \times \hat{e}_{oE})] \int_A (1-e^{-i\Phi}) e^{iks\sin\theta(\xi\cos\phi+\eta\sin\phi)} d\xi d\eta \quad (33)$$

where  $\hat{e}_k$  is a unit vector in the direction of observation. From a consideration of Figure 2,  $\hat{e}_k$  can be written

$$\hat{e}_k = \sin\theta \cos\phi \hat{e}_1 + \sin\theta \sin\phi \hat{e}_2 + \cos\theta \hat{e}_3 \quad (34)$$

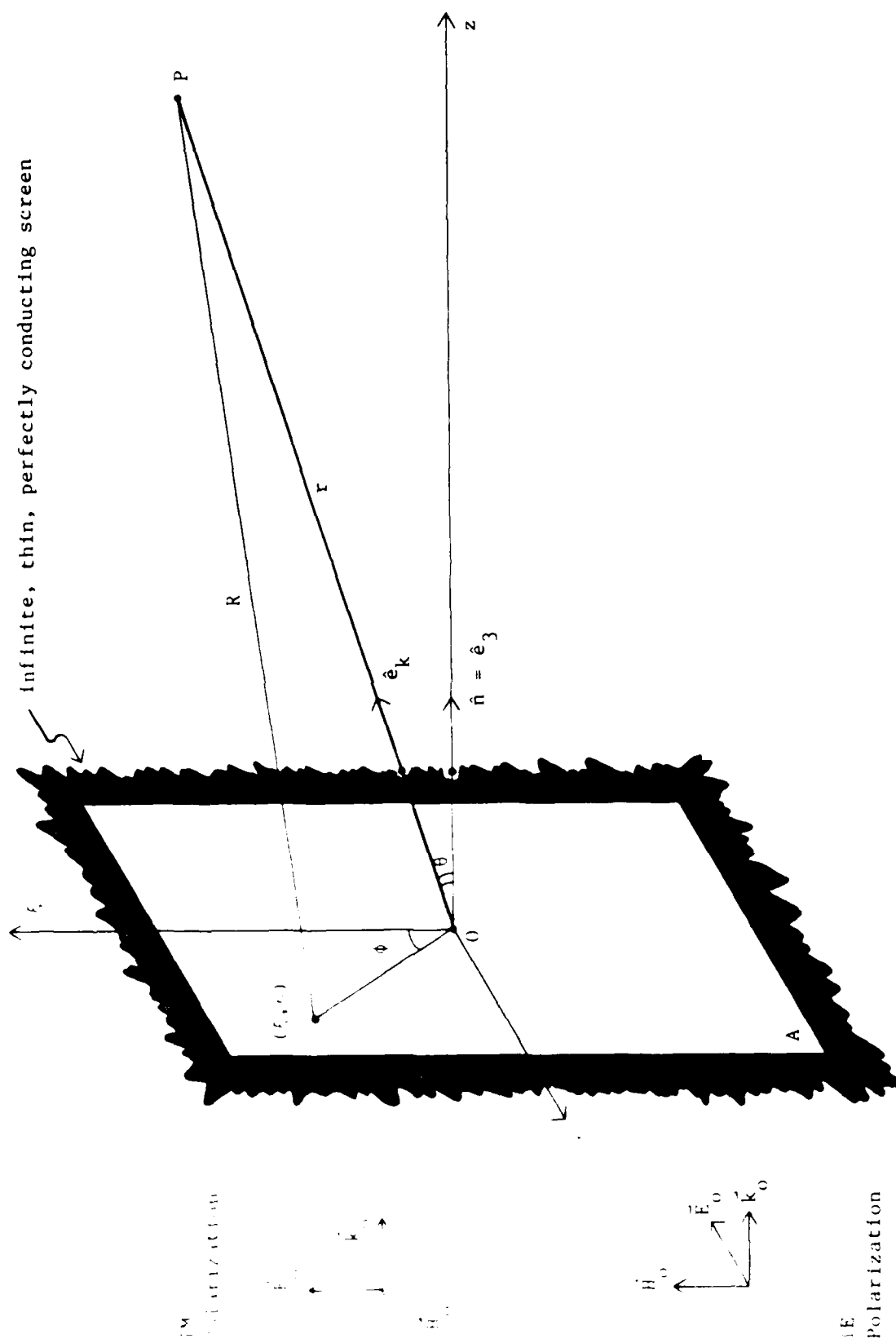
Now, we must consider the two polarization states. For TM polarization  $\hat{e}_{oE} = \hat{e}_1$ ; for TE polarization,  $\hat{e}_{oE} = -\hat{e}_2$ . For either case, only the factor  $[\hat{e}_k \times (\hat{e}_3 \times \hat{e}_{oE})]$  is affected in equation (33), so I will give the remainder of the equation the designation  $k(F)^{\frac{1}{2}}$ . From equation (17), for the TM case we find

$$\frac{dC_{sca}}{d\Omega} = F [\sin^2\theta \cos^2\phi + \cos^2\theta] \quad (35)$$

For the TE case, we get

$$\frac{dC_{sca}}{d\Omega} = F [\sin^2\theta \sin^2\phi + \cos^2\theta] \quad (36)$$

Figure 2. The geometry to be considered when making calculations of the diffraction of a polarized wave by a rectangular aperture (A) located in a thin, perfectly conducting, infinite screen.



An inspection of (35) and (36) shows that  $dC_{sca}/d\Omega$  is predicted to be polarization dependent. However, if we recall that in equation (16) we required  $\theta$  to be small, then  $\sin \theta \approx \theta$ , and  $\sin^2 \theta$  is even smaller. Consequently, the first terms of both equations (35) and (36) are negligible within the limits of the approximation, thus  $dC_{sca}/d\Omega$  is no longer predicted to be polarization dependent.

### 2.2.2 Application of the Kirchhoff-Kottler Formula

Bouwkamp (1954) gave the details of the Kirchhoff-Kottler vector formulation of Huygen's principle in his excellent review of diffraction. When the scalar Kirchhoff formula is applied to the six field components, the six wave functions so obtained do not satisfy Maxwell's equations in general. Kottler noted that this difficulty could be overcome by introducing additional terms in the Kirchhoff formula representing the effects of fictitious line charges along the rim of the aperture. In this section, the Kirchhoff-Kottler relation will be used to modify anomalous diffraction. It is hoped that Kottler's improvements of the Kirchhoff relation will allow for the prediction of polarization dependent extinction and differential scattering cross sections.

Again, we need to know  $\vec{S}(0)$ . Appendix B provides the details of the derivation of  $\vec{S}(0)$  from the Kirchhoff-Kottler relation. By analogy with van de Hulst, we generalize  $\vec{S}(0)$  to include rays transmitted through the cylinder, thus equation (57) becomes

$$\begin{aligned} \vec{S}(0) = & \frac{-k^2}{4\pi} \{ [\hat{e}_3 \times (\hat{e}_3 \times \hat{e}_{oE})] \\ & - [\hat{e}_3 \times (\hat{e}_3 \times (\hat{e}_3 \times (\hat{e}_3 \times \hat{e}_{oE}))) \} \int_A (1 - e^{-i\phi}) d\xi d\eta \end{aligned} \quad (37)$$

As with the Kirchoff modification of anomalous diffraction, the substitution of either the TM or TE polarizations into equations (27) and (31) gives identical values of  $U_{\text{ext}}$  so, even the improvements of Kottler fail to properly account for the polarization dependence of  $U_{\text{ext}}$ .

To calculate the differential scattering cross section, we proceed as in section 2.2.2 to get

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{-k^2}{4\pi} \left[ (1 + \cos^2 \theta) (\hat{e}_k \times \hat{e}_i \cdot \hat{e}_s + \hat{e}_i \cdot \hat{e}_s) \right. \\ &\quad \left. + (\hat{e}_k \times \hat{e}_i \cdot \hat{e}_s + \hat{e}_k \times \hat{e}_s \cdot \hat{e}_i) \right] \\ &= \frac{k^2}{4\pi} (1 + \cos^2 \theta) \sin^2 \theta \sin^2 \phi + \sin^2 \theta \sin^2 \phi \end{aligned} \quad (32)$$

As before, we must consider both the TE and TM polarization cases. Since the factor in the brackets is the only one dependent on  $\theta$ , designate the remainder of the equation as  $k^2 F$ . As reported in (32) and (33) will show that  $F = 2F_1$ . From equation (32), for the TM case ( $\hat{e}_{oE} = \hat{e}_i$ ) we get

$$\frac{d\sigma_{\text{TM}}}{d\Omega} = F_1^2 (\cos^2 \theta + \sin^2 \theta \sin^2 \phi + \cos^2 \theta + \sin^2 \theta \sin^2 \phi) = 4F_1^2$$

$$F_1 = \sin \theta \cos \theta \cos \phi + \sin \theta \cos \phi \quad (33)$$

For the TE case ( $\hat{e}_{oE} = -\hat{e}_i$ ), we get

$$\begin{aligned} \frac{d\sigma_{\text{scat}}}{d\Omega} = & E^2 \left[ \cos^2 \theta + \sin^2 \theta \cos^2 \phi + \cos^2 \theta \sin^2 \phi + \sin^4 \theta \sin^2 \phi \cos^2 \phi + \right. \\ & \left. 2 \sin^2 \theta \cos \theta \sin \phi + \sin^4 \theta \sin \phi \right]^2 \end{aligned} \quad (40)$$

As a section,  $\frac{d\sigma_{\text{scat}}}{d\Omega}$  is predicted to be polarization dependent. However, if we again neglect terms containing factors of order  $\sin^2 \theta$  and  $\sin^4 \theta$ , both equations (39) and (40) reduce to the following:

$$\frac{d\sigma_{\text{scat}}}{d\Omega} = E^2 \left[ \cos^2 \theta + \cos^2 \theta \right]^2 = \frac{E^2}{4} (\cos^2 \theta + \cos^2 \theta)^2 \quad (41)$$

Therefore, as for the Kirchhoff vector modification of anomalous scattering, within the limits of the approximation, the differential scattering cross section is not predicted to be polarization dependent.

## Chapter 3

### CONCLUSIONS

The extinction efficiency and differential scattering cross section of a cylinder at normal incidence were calculated with vector-modified anomalous diffraction expressions. In one case, the modification was based on the Kirchhoff vector formulation of Huygen's principle. In another case, the modification was based on the Kirchhoff-Kottler vector formulation of Huygen's principle. In neither case did the modification enable the polarization dependency of  $Q_{\text{ext}}$  to be predicted. In both cases, the polarization dependence of  $dC_{\text{sca}}/d\Omega$  was predicted, but within the limits of the approximation, i.e., for small angle light scattering, the polarization dependence vanished. In conclusion, both modifications of anomalous diffraction must be considered failures since no new information is gained with the added complexity.

The fundamental deficiency of both methods seems to lie in the Kirchhoff assumption that the exact fields at the diffracting obstacle can be replaced by the unperturbed incident field. This assumption seems reasonable in light of the anomalous diffraction assumption that  $|m-1| \ll 1$ . If some knowledge of the exact functional form of the fields at the diffracting obstacle could be obtained, perhaps the polarization dependence of the extinction efficiency and differential scattering cross sections could be found in a simple way. However, I doubt that the resulting expressions would maintain the simplicity that makes anomalous diffraction so useful.



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APPENDIX A

RELATION OF  $\bar{S}$  FROM THE  
KIRKWOOD DIFFRACTION RELATION

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THE APPLICATION OF VECTOR DIFFRACTION TO THE SCALAR  
ANOMALOUS DIFFRACTION. (U) AIR FORCE INST OF TECH  
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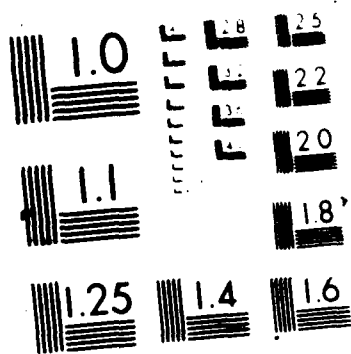
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Jackson (1975, p. 438) provided the expression, derived from Kirchhoff's vector formulation of Huygen's principle, for the field diffracted by an aperture located in a thin, perfectly conducting screen. Assuming the radiation is incident from the  $-z$  direction and that the aperture is in the  $z = 0$  plane, it is

$$\vec{E}_D = \frac{1}{2\pi} \vec{\nabla} \times \int_A [\hat{n} \times \vec{E}]_{z=0} \frac{e^{ikR}}{R} d\xi d\eta \quad (46)$$

where  $\vec{E}_D$  is the diffracted field in the region  $z > 0$ ,  $\vec{\nabla}$  is the three-dimensional del operator,  $\hat{n}$  is a unit normal on the aperture pointing into the space  $z > 0$ ,  $\vec{E}$  is the field in the plane  $z = 0$ ,  $R$  is the distance from a source point on the aperture to the observation point  $P$ , and  $\xi$  and  $\eta$  are source-point coordinates in the aperture. The integration is taken over the aperture area, and the del operator is applied to the source-point coordinates.

If the observation point is located far from the aperture ( $kR \gg 1$ ), then  $kR$  can be expanded as

$$kR = kr - k\hat{e}_k \cdot \vec{r}' + \text{h.o.t.} \quad (47)$$

where  $r$  is the distance from the origin (assumed to be located somewhere in the aperture) to the observation point,  $\hat{e}_k$  is a unit vector in the direction of observation, and  $\vec{r}'$  is a vector from the origin to the source-point. If we neglect the higher order terms (h.o.t.), then we are considering Fraunhofer diffraction.

Consider Figure 2. The aperture area is equal to the projected area of the cylinder under consideration. From the definitions of  $\theta$  and  $\phi$  in the figure, we can rewrite (47) as

$$kR = kr - k\sin\theta(\xi\cos\phi + \eta\sin\phi) \quad (48)$$

If we substitute (48) into (46) along with the usual Kirchhoff assumption that the field in the aperture can be approximated by the unperturbed incident field, i.e.,  $\vec{E} = E_o \hat{e}_{oE}$ , we get

$$\vec{E}_D = \frac{E_o e^{ikr}}{ikr} \vec{S}(\theta, \phi) \quad (49)$$

where

$$\vec{S}(\theta, \phi) = \frac{-k^2}{2\pi} [\hat{e}_k \times (\hat{e}_3 \times \hat{e}_{oE})] \int_A e^{-ik\sin\theta(\xi\cos\phi + \eta\sin\phi)} d\xi d\eta \quad (50)$$

is the vector scattering amplitude and where  $\hat{e}_{oE}$  is a unit vector in the direction of polarization of the incident electric vector.

Equation (50) applies to an aperture, but we are interested in diffraction by a cylinder. Babinet's principle for an electromagnetic wave states that the diffraction of a TE wave by an aperture is equivalent to the diffraction of a TM wave by the aperture's complement. Therefore, once the aperture diffraction problem is solved for both polarization cases, the complementary problem is also solved. Furthermore, we will assume that within the limits of the approximation, the diffraction pattern of a perfectly opaque cylinder is equal to that of a thin, perfectly conducting screen equal to the cylinder's projected area.

To calculate the extinction efficiency, we need to know  $\vec{S}(0)$ , the vector forward scattering amplitude. As  $\theta \rightarrow 0$ ,  $\hat{e}_k \rightarrow \hat{e}_3$  and (50) becomes

$$\vec{S}(0) = \frac{-k^2}{2\pi} [\hat{e}_3 \times (\hat{e}_3 \times \hat{e}_{oE})] \int_A d\xi d\eta \quad (51)$$

## APPENDIX B

CALCULATION OF  $\vec{S}(0)$  FROM THE KIRCHOFF-KOTTLER  
VECTOR DIFFRACTION RELATION

Bouwkamp (1954, p. 58) provided the expression, derived from the Kirchhoff-Kottler formulation of Huygen's principle, for the field diffracted by an aperture located in a thin, perfectly conducting screen. Assuming the radiation is incident from the  $-z$  direction and that the aperture is located in the plane  $z = 0$ , it is

$$\begin{aligned}\vec{E}_D &= \vec{\nabla} \times \frac{1}{4\pi} \int_A [\hat{n} \times \vec{E}]_{z=0} \frac{e^{ikR}}{R} d\xi d\eta \\ &\quad - \vec{\nabla} \times \vec{\nabla} \times \frac{1}{4\pi ik} \int_A [\hat{n} \times \vec{H}]_{z=0} \frac{e^{ikR}}{R} d\xi d\eta\end{aligned}\quad (52)$$

where the variables are equal to those of Appendix A.

All of the general considerations of Appendix A and Figure 2 will again be used here. For an incident plane wave with the fields given by  $\vec{E}_0 = E_0 \hat{e}_{0E}$  and  $\vec{H}_0 = H_0 \hat{e}_{0H}$ , the fields are related by

$$\vec{H}_0 = \frac{1}{k} [\vec{k}_0 \times \vec{E}_0] \quad (53)$$

where  $\hat{e}_{0E}$  and  $\hat{e}_{0H}$  are unit vectors in the direction of polarization of the incident electric and magnetic vectors, respectively, and  $\vec{k}_0 = k\hat{e}_3$  is the incident wave vector. As before, the values of the fields in the aperture are taken to be those of the unperturbed incident wave; also, the Fraunhofer limit is taken to get

$$\vec{E}_D = \frac{E_0 e^{ikr}}{ikr} \vec{S}(\theta, \phi) \quad (54)$$



where

$$\begin{aligned} \vec{S}(\theta, \phi) = & \frac{-k^2}{4\pi} \{ [\hat{e}_k \times (\hat{e}_3 \times \hat{e}_{oE})] \\ & - [\hat{e}_k \times (\hat{e}_k \times (\hat{e}_3 \times (\hat{e}_3 \times \hat{e}_{oE})))] \} \int_A e^{i\vec{k} \cdot \vec{r}'} d\xi d\eta \quad (55) \end{aligned}$$

and where

$$\vec{k} \cdot \vec{r}' = k \sin \theta (\xi \cos \phi + \eta \sin \phi) \quad (56)$$

Babinet's principle is applied as in Appendix A.

Again, we desire to know  $\vec{S}(0)$ . Analogously with Appendix A, as

$\theta \rightarrow 0$ ,  $\hat{e}_k \rightarrow \hat{e}_3$ , and consequently

$$\begin{aligned} \vec{S}(0) = & \frac{-k^2}{4\pi} \{ [\hat{e}_3 \times (\hat{e}_3 \times \hat{e}_{oE})] \\ & - [\hat{e}_3 \times (\hat{e}_3 \times (\hat{e}_3 \times (\hat{e}_3 \times \hat{e}_{oE})))] \} \int_A d\xi d\eta \quad (57) \end{aligned}$$

END

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